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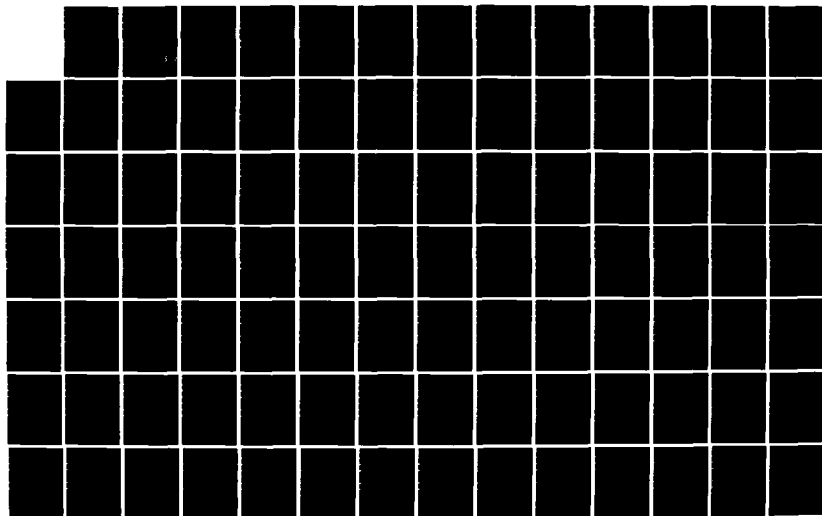
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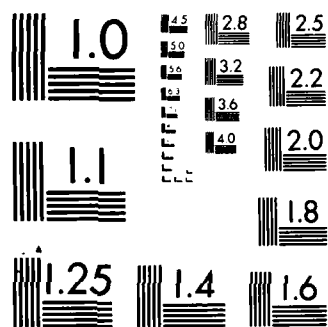
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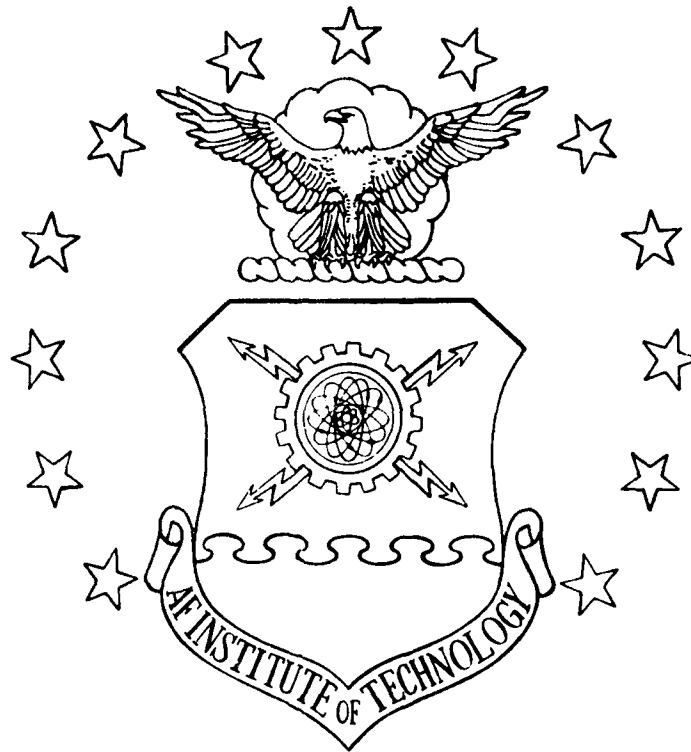
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A FINITE ELEMENT SOLUTION OF THE  
TRANSPORT EQUATION

THESIS

Frederick A. Tarantino  
Captain IN, USA

AFIT/GNE/PH/85M-19

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A FINITE ELEMENT SOLUTION OF THE  
TRANSPORT EQUATION

THESIS

Presented to the Faculty of the School of Engineering of  
the Air Force Institute of Technology  
Air University

In Partial Fulfillment of the Requirement for  
the Degree of Master of Science in Nuclear Science

Frederick A. Tarantino B.S.

Captain IN, USA

March 1985

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TRANSPORT EQUATION

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### Abstract

Using a self adjoint form of the transport equation expressed as a variational integral, finite element equations for the one dimensional, one speed, homogeneous, time independent transport equation in slab geometry were derived and encoded in Fortran 77. The accuracy of  $C_0$  and  $C_1$  continuous fits was compared against an analytical solution for the case of noscatter. It was found that the  $C_0$  fits require an excessive amount of mesh refinement. The  $C_1$  fit is very accurate, and does not appear to be computationally excessive.

The finite element results were then compared, for the case of isotropic scatter, to a legendre polynomial solution, and the results of a recently developed code known as Ln. The methods accuracy was sufficiently verified with inexact scattering term evaluation. A technique of exact scattering integral evaluation is proposed that should reduce the amount of refinement required for convergence, and improve computational efficiency.

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## Preface

The purpose of this study was to continue the work of a previous graduate student, (A.D. Goff GNE 84M) and demonstrate that a finite element solution of the transport equation would work. Using a self adjoint form of the transport equation expressed as a variational integral, finite element equations with  $C^0$  and  $C^1$  continuity were derived, encoded and compared to a spherical harmonic solution over a test case domain.

I have been extremely pleased with the graduate education provided by the AFIT GNE faculty. Dr.'s Charles Bridgman , George John and Bernard Kaplan all deserve my thanks. I would particularly like to thank Dr. Donn Shankland for his guidance and instruction throughout this study. He provided a challenging and exciting thesis topic, from which I have learned greatly. Finally I would like to thank my wife Jazmine, whose love and understanding never falter.

Frederick A. Tarantino

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## Notation

### Coordinates

- $x, y, z$  - Cartesian coordinates  
 $l_1, l_2, l_3$  - Triangular coordinates  
 $L_1, L_2, L_3, L_4$  - Tetrahedral coordinates

### Operators

- $d$  - Derivative  
 $\partial$  - Partial derivative  
 $\nabla$  - Gradient  
 $\delta$  - First variation  
 $L$  - SATE operator  
 $+$  - Adjoint  
 $\sim$  - Transpose  
 $\mathcal{L}$  - Transport operator  
 $\Sigma$  - Summation  
 $!$  - Factorial

### Variables

- $\phi$  - Angular flux  
 $\Sigma_t$  - Total macro cross section  
 $\Sigma_s$  - Isotropic cross section for scatter  
 $\mu$  - Direction cosine in 1-D, before collision  
 $\mu'$  - Direction cosine in 1-D, after collision  
' - Primed refers to after-collision properties  
- Unprimed refers to before-collision coordinates  
 $I$  - Variational functional

$A$  - Area

$V$  - Volume

#### Matrices

$\underline{\underline{MG}}$  - Global matrix

$\underline{\underline{GT}}$  - Matrix of interpolating function constants

$\underline{\underline{I}}$  - Identity matrix

$\underline{\underline{MA}}$  - Absorbing matrix

$\underline{\underline{MS}}$  - Streaming matrix

$\underline{\underline{MB}}$  - Boundary matrix

$\underline{\underline{ML}}$  - Local matrix

$\underline{\underline{NML}}$  - Non local matrix

$\underline{\underline{O}}$  - Zero matrix

$\underline{\underline{LI}}$  - Local integral

$\underline{\underline{NLI}}$  - Non local integral

#### Vectors

$\underline{h}$  - Basis functions

$\underline{m}$  - Vector of natural coordinate polynomials, which together constitute a complete basis, of first, second or third order depending upon the fit being used.

$\underline{\varphi}$  - Vector of finite element interpolating nodes

$\underline{f}$  - Vector of product  $\phi\phi'$

$\underline{g}$  - Vector of product  $\phi_x\phi'$

$(1,0,0)$ ,  $\Phi = \varphi_2$  at node 2, and  $\Phi = \varphi_3$  at node 3. This fit has  $C^0$  continuity since flux is continuous along element interfaces, but its first partial derivatives are not.

The quadratic fit for this element requires six degrees of freedom.

$$\Phi = \sum_{i=1}^6 h_i \varphi_i' \quad (2-12)$$

Where the  $h_i$  are basis functions and the  $\varphi_i'$  are now the value of the flux at corner nodes and the first derivative with respect to  $\gamma$ . Such that

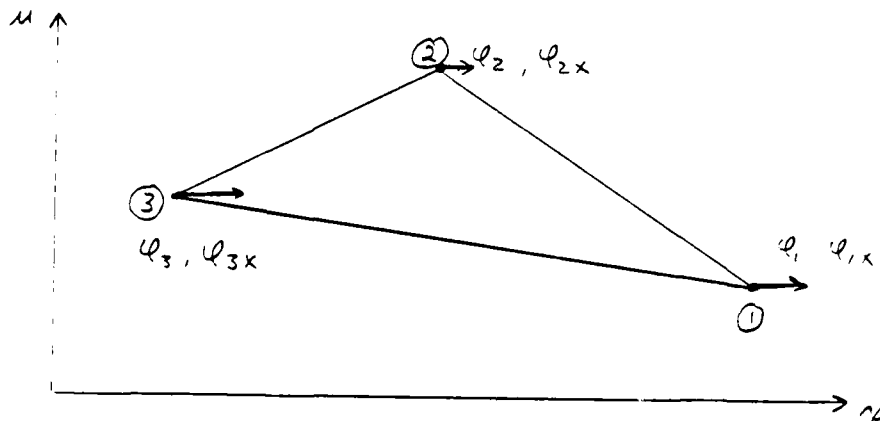


Figure 2-2  
Quadratic Fit Using Derivatives at  
Corner Nodes

$$\Phi = \tilde{h} \underline{\varphi} \quad (2-13)$$

where

$$\tilde{h} = \begin{bmatrix} h_1 & h_2 & h_3 & h_{1x} & h_{2x} & h_{3x} \end{bmatrix} \quad (2-14)$$

and

$$\frac{\partial \Phi(1,0,0)}{\partial x} = h_{1x} \quad \frac{\partial \Phi(0,1,0)}{\partial x} = h_{2x} \quad \frac{\partial \Phi(0,0,1)}{\partial x} = h_{3x}$$

node 2 is at (0,1,0) and node 3 at (0,0,1) .

Over the area of a triangle the integral of natural coordinate powers is given (3:145) by

$$\int \Delta l_1^p l_2^q l_3^r = 2A \frac{p! q! r!}{(p+q+r+2)!} \quad (2-7)$$

where  $A$  is the area of the triangle and is equal to

$$2A = \begin{vmatrix} 1 & 1 & 1 \\ \eta_1 & \eta_2 & \eta_3 \\ \mu_1 & \mu_2 & \mu_3 \end{vmatrix} \quad (2-8)$$

The simplest interpolant for a triangle is the linear fit. It express the field variable,  $\Phi$ , (in this case particle angular flux) across the triangle as a linear combination of the flux at the corner nodes such that

$$\Phi = \Phi(x, \mu) = \Phi(\eta, l_2, l_3) = \sum_{i=1}^3 l_i \varphi_i \quad (2-9)$$

The partial derivatives of the flux are

$$\frac{\partial \Phi}{\partial x} = \sum_{i=1}^3 \frac{\partial l_i}{\partial x} \varphi_i = \sum_{i=1}^3 g_i \varphi_i \quad (2-10)$$

$$\frac{\partial \Phi}{\partial \mu} = \sum_{i=1}^3 \frac{\partial l_i}{\partial \mu} \varphi_i = \sum_{i=1}^3 f_i \varphi_i \quad (2-11)$$

where  $g_i$  and  $f_i$  are the partial derivatives of the three natural coordinates with respect to  $\eta$  and  $\mu$  respectively. Within an element they are constant, but are different for each distinct triangle geometry. Note that  $\frac{\partial \varphi_i}{\partial x} = \frac{\partial \varphi_i}{\partial \mu} = 0$

It is clear from this expression that the equation is satisfied at corner nodes, that is that  $\Phi = \varphi_i$ , at node 1

element (3:140). In two dimensions this system is often referred to as area coordinates, since it can easily be shown that the natural coordinates represent ratios of area.

Over a triangle one expresses the  $(x, u)$  coordinates in terms of three variables  $l_1$ ,  $l_2$  and  $l_3$  such that the sum of the natural coordinates is always one.

$$l_1 + l_2 + l_3 = 1 \quad (2-1)$$

The linear relation below exists between the cartesian and natural coordinates;

$$l_1 x_1 + l_2 x_2 + l_3 x_3 = x \quad (2-2)$$

$$l_1 u_1 + l_2 u_2 + l_3 u_3 = u \quad (2-3)$$

Written in matrix form the above relations become

$$\begin{bmatrix} 1 & 1 & 1 \\ x_1 & x_2 & x_3 \\ u_1 & u_2 & u_3 \end{bmatrix} \begin{bmatrix} l_1 \\ l_2 \\ l_3 \end{bmatrix} = \begin{bmatrix} 1 \\ x \\ u \end{bmatrix} \quad (2-4)$$

It is easily shown from this expression that

$$\frac{\partial l_1}{\partial x} = \frac{u_2 - u_3}{2 (\text{Area of triangle})} \quad (2-5)$$

and

$$\frac{\partial l_1}{\partial u} = \frac{x_3 - x_2}{2 (\text{Area of triangle})} \quad (2-6)$$

and that the indices permute cyclically. Note that the coordinates of node 1 in figure 2-1 are  $(l_1, l_2, l_3) = (1, 0, 0)$

compatibility requirement of elements. Without it, "gaps" may arise between elements from discontinuous derivatives, and unsolicited contributions to field variables can arise. Completeness is the term associated with the second requirement. It insures that the variational integral is well defined.

Standard finite element nomenclature is to express element continuity as a function of the highest order derivative held continuous on boundaries.  $C^0$  continuity implies field variable values are continuous on element edges,  $C^1$  continuity has variable and first derivative inter-element continuity, and so on.

#### B. The Triangle and Two Dimensional Interpolating Functions

The two dimensional element chosen for this study was the triangle. It is a simple element to refine, can be maneuvered easily to snugly fit irregular boundaries, and can be expediently described in terms of its natural coordinates

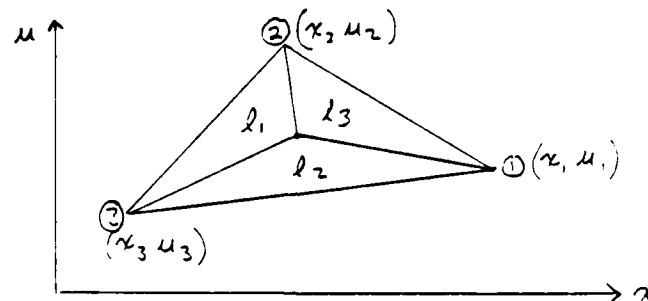


Figure 2-1  
Cartesian and Triangular Coordinates

A natural coordinate system is a local coordinate system that relies upon the element geometry for its definition, and whose coordinates range in value from zero to one within an

## 2. Elements and Interpolating Functions

The study of interpolating functions, and the elements composing finite element meshes is an important one. The wrong choices can cause excessive computations, or worse prevent convergence from occurring. The elements and interpolating functions presented here are by no means inclusive. Finite element literature on the topic is extensive.

In this section general requirements for monotonic convergence of the finite element method will be presented. Then, the two and three dimensional elements chosen for this study are described. Finally the interpolating functions used for each element are given, and their derivations are explained.

### A. Compatibility and Completeness

Convergence of the finite element method is guaranteed if the elements composing the mesh, and the selected interpolation function satisfy two requirements (3:79). Namely, 1) along element boundaries the field variable and any of its partial derivatives up to one order less than the highest order derivative appearing in the variational functional must be continuous and 2) the field variable, and its partial derivatives up to the highest order appearing in the functional should be represented in the interpolation function as the limit of element size approaches zero.

The first of these requirements is the so called

variable value at that node must be the same from each element possessing that node.

5) Solve the System Equations. The resulting coefficient matrix (referred to as the global matrix) is symmetric, banded and positive definite. System of equations with coefficient matrices of this type are best solved by Cholesky decomposition (7:13) and it is the algorithm used in this study. Solution of the system equations yields nodal values of the field variable, which together with the interpolating function defines piecewise approximations across the domain under scrutiny.

6) Make additional Computations if desired. With respect to the transport equation this step is not required, except in the case where penalties are desired for automatic mesh refinement.

#### D) Summary

Operating on the transport operator with the adjoint transport operator produces a self adjoint transport equation. This equation can be expressed variationally as a quadratic functional, that when minimized is equivalent to solving the SATE. The finite element method is best suited for solving this type of problem. It is a numerical technique that approximates field variable values with separate analytical expressions, of the same order, across a mesh of small interconnected elements. The resulting set of linear equations is positive definite, and can be solved quickly by direct means.

in step 3 below. Additionally, triangles are easily generated and refined, and fit irregular boundaries snugly. In general one should start with a sparse mesh composed of few elements. This allows a solution to be calculated, and regions of high penalty identified for mesh refinement. Constructing large meshes by hand is a time consuming and error prone process. References for automatic mesh generation are listed in Heubner (3:511).

2) Select interpolation functions. Chapter two is dedicated to this topic. Interpolating nodes must be assigned to each element, and interpolants chosen. The form of these functions depend upon the number of geometric nodes an element possesses, the number of unknowns at each node, and certain continuity requirements to be discussed in section 2-a.

3) Find the element properties. The interpolation functions are substituted for the field variable in the functional, and the integral is evaluated. When the resultant expressions are minimized with respect to nodal values, the remaining matrix equation describes element properties in terms of nodal variables. Element properties are expressed in terms of the coefficient matrices of this equation, referred to in this report as the local and nonlocal matrices.

4) Assemble element properties to obtain system equations. When local and nonlocal matrices are computed for each element, they are assembled globally to provide a set of simultaneous linear equations with nodal values as the unknowns. The foundation for this procedure lies on the fact that if a node is shared by more than one element the field

than a finite difference rectangular grid. An additional advantage of the method is that mesh refinement can occur easily, and that there is a built-in indicator to dictate where mesh refinement should occur. Local mesh refinement, cumbersome in a finite difference grid, consists only of subdividing a finite element into smaller ones. Elements over which this is necessary are discovered by evaluating the so-called penalty function. Since the variational integral is minimized, its value over a particular element is referred to as that element's penalty. Elements where large penalties occur are those where the interpolation function fit is poorest, and mesh refinement is required. These elements can be subdivided until penalties are equal across the mesh and further refinement fails to produce significant total penalty reduction.

#### Solution steps

These six steps are given by Heubner (3:7) as an orderly method for obtaining a finite element solution. They are described in general terms below, and are elaborated upon specifically with respect to the SATE in later sections.

- 1) Discretize the Continuum. The first step is to divide the domain under consideration into a set of interconnected elements. A multififormity of elements may be used. The triangle is very well suited for two dimensional problems, and it is the element used in this study. The ability to express interpolating functions in terms of triangular natural coordinates simplifies the evaluation of integrals appearing

Across each of these elements an assumed solution is prescribed, called an interpolating, or approximating function. This solution is written as a function of field variable values, and sometimes the variable's spatial derivatives, at element nodes. Solution requires choosing these nodal variables so as to minimize the variational statement of the problem and satisfy boundary conditions. If the operator acting upon the field variable is self-adjoint, then equations describing the variable values at element nodes can be assembled globally, (over the entire material) and an approximate solution to the partial differential equation can be calculated by solving the resulting set of simultaneous linear equations.

Consider a comparison of the finite element method with the well known finite difference method. The finite difference approximation is that a derivative can be approximated by a difference operation over a very small interval. The resulting solution is a set of grid points at which the field variable values are defined. Finite elements assumes an analytical expression for variable values over a small element. This approach results in a piecewise approximation, with field variable values given by separate analytic expressions across an array of small, interconnected elements, as well as at interpolation nodes.

Because the finite element mesh is composed of elements, they can be put together in a variety of ways. This makes the method well suited for problems with complex geometries. Small elements can be made to fit an irregular boundary much easier

$$\begin{aligned}
I &= \frac{1}{2} \int_D \left\{ \mu \frac{\partial \phi}{\partial x} + \varepsilon_t \phi - \frac{\varepsilon_s}{2} \int_{-1}^1 du' \phi' \right\}^2 dx \\
I &= \frac{1}{2} \int_D \left\{ \mu^2 \left( \frac{\partial \phi}{\partial x} \right)^2 + \varepsilon_t^2 \phi^2 + 2\mu \varepsilon_t \frac{\partial \phi}{\partial x} \phi \right. \\
&\quad + \left( \frac{\varepsilon_s}{2} \int_{-1}^1 du' \phi' \right) \left( \frac{\varepsilon_s}{2} \int_{-1}^1 du'' \phi'' \right) - \mu \varepsilon_s \frac{\partial \phi}{\partial x} \int_{-1}^1 du' \phi' \\
&\quad \left. - \varepsilon_t \varepsilon_s \phi \int_{-1}^1 du' \phi' \right\} dx \quad (1-16)
\end{aligned}$$

To be sure this is correct, the expressions given by equations (1-9) and (1-10) should be satisfied. Specifically

$$\frac{\partial (\mathcal{L}\phi)^2}{\partial \phi} - \frac{\partial}{\partial x} \frac{\partial (\mathcal{L}\phi)^2}{\partial \phi_x} = 0 \quad (1-17)$$

should reduce to the self adjoint transport equation, and

$$\frac{\partial (\mathcal{L}\phi)^2}{\partial \phi_x} = 0 \quad (1-18)$$

is the condition required along the boundary. Straightforward substitution verifies that (1-17) is the SATE, and that the natural boundary condition is the transport equation itself, certainly an acceptable requirement.

Up to this point the transport equation has been recast into a variational form, and it has been shown that minimizing this functional is equivalent to solving the SATE. In the next section is presented background on a numerical technique which has achieved the most success in solving this type of problem.

### C) The Finite Element Method

The finite element method is a numerical technique used to solve partial differential equations. The region under scrutiny is divided up into a finite number of elements.

$$I = \frac{1}{2} \int_D (\mathcal{L}\phi - s)(\mathcal{L}\phi - s) dD \quad (1-11)$$

yields

$$I = \frac{1}{2} \int_D (\mathcal{L}\phi\mathcal{L}\phi - 2s\mathcal{L}\phi + s^2) dD \quad (1-12)$$

Using the definition of adjointness this functional can be expressed as

$$I = \frac{1}{2} \int_D (\phi\mathcal{L}^*\mathcal{L}\phi - 2\phi\mathcal{L}^*s + s^2) dD \quad (1-13)$$

Setting the variation equal to zero, using the definition of adjointness and recalling that  $\mathcal{L}^*\mathcal{L}$  is self adjoint gives

$$\delta I = \frac{1}{2} \int_D \{ \delta\phi(\mathcal{L}^*\mathcal{L}\phi - 2\mathcal{L}^*s) + \phi\mathcal{L}^*\mathcal{L}\delta\phi \} dD$$

$$\delta I = \int_D \delta\phi(\mathcal{L}^*\mathcal{L}\phi - \mathcal{L}^*s) dD = 0$$

$$\delta I = \int_D \delta\phi \mathcal{L}^*(\mathcal{L}\phi - s) dD = 0 \quad (1-14)$$

Solution of which is identical to solving the SATE.

#### The One Speed, One Dimensional Functional

The one dimensional, one speed, time independent transport equation is given (1:76) by

$$\mu \frac{\partial \phi}{\partial x} + \Sigma_t \phi = \frac{\Sigma_s}{2} \int_{-1}^1 du' \phi(x, u') \quad (1-15)$$

in the case of isotropic scatter, with no sources, where

$\mu$  = cosine(angle particle is traveling)

$\phi = \phi(x, \mu)$  , angular flux

$\Sigma_s$  = scattering cross section

In this case  $\mathcal{L} = \mu \frac{\partial}{\partial x} + \Sigma_t - \frac{\Sigma_s}{2} \int_{-1}^1 du'$

This is the form of the transport equation chosen to test the finite element solution of the quadratic transport functional. The expression requiring minimization now becomes

where  $\phi = \phi(x, u)$ .

The minimum of this functional is found in an analogous manner to finding the minimum of a function in ordinary calculus, by setting the variation to zero.

$$\delta I = \int_{u_1}^{u_2} \int_{x_1}^{x_2} \left[ \frac{\partial F}{\partial \phi} \delta \phi + \frac{\partial F}{\partial \phi_x} \delta \phi_x \right] dx du = 0 \quad (1-7)$$

Integrating the second term by parts

$$\int \omega dv = v\omega - \int v d\omega$$

$$\omega = \frac{\partial F}{\partial \phi_x} \quad v = \delta \phi$$

$$d\omega = \frac{\partial}{\partial x} \frac{\partial F}{\partial \phi_x} dx \quad dv = \delta \phi_x dx$$

gives

$$\delta I = \int_{u_1}^{u_2} \int_{x_1}^{x_2} \left[ \frac{\partial F}{\partial \phi} - \frac{\partial}{\partial x} \frac{\partial F}{\partial \phi_x} \right] \delta \phi dx du + \int_{u_1}^{u_2} \frac{\partial F}{\partial \phi_x} \delta \phi \Big|_{x_1}^{x_2} \quad (1-8)$$

Since  $\delta \phi$  is an arbitrary admissible variable (H:551)  $\delta I$  can equal zero only if

$$\frac{\partial F}{\partial \phi} - \frac{\partial}{\partial x} \frac{\partial F}{\partial \phi_x} = 0 \quad (1-9)$$

and

$$\frac{\partial F}{\partial \phi_x} \Big|_{x_1}^{x_2} = 0 \quad (1-10)$$

The first term above is a simplified version of the Euler-Lagrange equation (3:551) and is the differential equation satisfied when  $I$  is minimized. The second expression is referred to as a natural boundary condition, since it specifies the solution form on the boundary, and since the functional can only be minimized when it is satisfied.

#### The Transport Functional

Expansion of the quadratic functional (2:15)

repeated here for the purpose of document continuity.

#### The Self-Adjoint Transport Equation (SATE)

Adjointness is defined (5:10) by the property

$$\int_D \phi \mathcal{L} \psi dD = \int_D \psi \mathcal{L}^+ \phi dD \quad (1-4)$$

where  $\mathcal{L}^+$  is the adjoint of the operator  $\mathcal{L}$ . If  $\mathcal{L} = \mathcal{L}^+$  then  $\mathcal{L}$  is said to be self-adjoint.

Consider the operator  $\mathcal{L} = \mathcal{L}^+ \mathcal{L}$  where  $\mathcal{L}$  is the transport operator and  $\mathcal{L}^+$  is its adjoint. Since

$$\begin{aligned} \int_D \phi \mathcal{L} \psi dD &= \int_D \phi \mathcal{L}^+ \mathcal{L} \psi dD = \int_D \mathcal{L} \psi \mathcal{L} \phi dD \\ &= \int_D \mathcal{L} \phi \mathcal{L} \psi dD = \int_D \psi \mathcal{L}^+ \mathcal{L} \phi dD = \int_D \psi \mathcal{L} \phi dD \end{aligned}$$

$\mathcal{L}$  is self adjoint. If  $\mathcal{L}^+$  is allowed to operate on the transport equation, the resultant expression

$$\mathcal{L}^+(\mathcal{L}\phi - s) = 0 \quad (1-5)$$

is self adjoint. Solutions of this equation must satisfy the transport equation (2:16).

$\mathcal{L}\phi - \mathcal{L}^+s = 0$  is a self adjoint operator equation, the solution of which always satisfies the transport equation. This expression is referred to as the self adjoint transport equation (SATE).

#### B) Variational Minimization of a Functional

The next task described in Goff's thesis was to find a variational functional, minimization of which would be equivalent to solving the SATE. Before reproducing that effort, consider the task of minimizing a functional,  $I(\phi)$ .

$$I = \int_{u_1}^{u_2} \int_{x_1}^{x_2} F(\phi, \phi_x) dx du \quad (1-6)$$

## 1. Introduction

### A) The Transport Equation

The Boltzman transport equation, written in its general integro-differential form is

$$\frac{1}{v} \frac{\partial \phi}{\partial t} + \hat{\Omega} \cdot \vec{\nabla} \phi + \Sigma_t \phi = S + \int_0^\infty dE' \int d\hat{\Omega}' \Sigma_s(E' \rightarrow E, \hat{\Omega}' \rightarrow \hat{\Omega}) \phi(r, E', \hat{\Omega}', t) \quad (1-1)$$

where

$v$  is particle velocity

$\phi$  is particle angular flux

$\hat{\Omega}$  is particle direction

$\Sigma_t$  is the transport cross section  $\Sigma_t(\vec{r}, \hat{\Omega}, E, t)$

$S$  is particle sources  $S(\vec{r}, \hat{\Omega}, E, t)$

$E$  is particle energy

$\Sigma_s(E' \rightarrow E, \hat{\Omega}' \rightarrow \hat{\Omega})$  is the scattering cross section from energy  $E'$  to  $E$  and angle  $\hat{\Omega}'$  to  $\hat{\Omega}$ . The transport equation can be written as

$$\mathcal{L} \phi - S = 0 \quad (1-2)$$

where the operator  $\mathcal{L}$  is clearly

$$\frac{1}{v} \frac{\partial}{\partial t} + \hat{\Omega} \cdot \vec{\nabla} + \Sigma_t - \int_0^\infty dE' \int d\hat{\Omega}' \Sigma_s(E' \rightarrow E, \hat{\Omega}' \rightarrow \hat{\Omega}) \quad (1-3)$$

In this formulation, the operator  $\mathcal{L}$  is non-self-adjoint. Finite element solutions of this equation have been tried (1 : 479) but without a self-adjoint operator, variational extremum principles do not exist, and the finite element method's power is not achieved.

Reformulating the transport operator into a self adjoint form has been accomplished (2:15) and its derivation is

The basis functions are found by requiring that at (1,0,0) = , and = . Four more identities are found by similar relations at nodes 2 and 3 . If the basis functions are considered to be the product

$$\underline{\hat{h}} = \underline{\hat{m}} \underline{G^T} \quad (2-15)$$

where

$$\underline{\hat{m}} = \begin{bmatrix} l_1^2 & l_2^2 & l_3^2 & l_1 l_2 & l_2 l_3 & l_1 l_3 \end{bmatrix} \quad (2-16)$$

is a matrix of polynomials, which together represent a complete quadratic basis, then

$$\phi = \underline{\hat{m}} \underline{G^T} \underline{\psi} \quad (2-17)$$

and

$$\frac{\partial \phi}{\partial x} = \phi_x = \frac{\partial \underline{\hat{m}}}{\partial x} \underline{G^T} \underline{\psi} \quad (2-18)$$

then since

$$\frac{\partial \underline{\hat{m}}}{\partial x} = \underline{\hat{m}}_x = \begin{bmatrix} 2l_1 g_1 & 2l_2 g_2 & 2l_3 g_3 & l_1 g_2 + l_2 g_1 & l_2 g_3 + l_3 g_2 & l_1 g_3 + l_3 g_1 \end{bmatrix} \quad (2-19)$$

the relation below must hold

$$\begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ g_1 & 0 & 0 & g_2 & 0 & g_3 \\ 0 & g_2 & 0 & g_1 & g_3 & 0 \\ 0 & 0 & g_3 & 0 & g_2 & g_1 \end{bmatrix} \underline{\underline{G}}^T = \underline{\underline{I}} \quad (2-20)$$

Where  $\underline{\underline{I}}$  is the identity matrix.

Finding  $\underline{\underline{G}}^T$  involves taking the inverse of the 6x6 matrix above. If this interpolating function matrix is partitioned into four 3x3 matrices, so that (2-20) can be written

$$\begin{bmatrix} \underline{\underline{I}} & \underline{\underline{O}} \\ \underline{\underline{A}} & \underline{\underline{B}} \end{bmatrix} \underline{\underline{G}}^T = \underline{\underline{I}} \quad (2-21)$$

then  $\underline{\underline{G}}^T$  can be found by

$$\underline{\underline{G}}^T = \begin{bmatrix} \underline{\underline{I}} & \underline{\underline{O}} \\ \underline{\underline{C}} & \underline{\underline{D}} \end{bmatrix} \quad (2-22)$$

where

$$\underline{\underline{C}} = \underline{\underline{B}}^{-1} \underline{\underline{A}} \quad (2-23)$$

and

$$\underline{\underline{D}} = \underline{\underline{B}}^{-1} \quad (2-24)$$

Now calculations are simplified since the inverse of only one 3x3 matrix must be found to invert the 6x6 interpolating function matrix. Flux at a point in the triangle is found by evaluating the matrix  $\underline{m}$  with the natural coordinates of the point in question, finding the derivatives of the natural coordinates in the triangle with respect to  $\chi$ , and calculating  $\underline{\omega}$ . Note that  $\underline{\omega}$  is a matrix of constants within a triangle, but since the  $g_i$  depend on triangle geometry,  $\underline{\omega}$  will also be different for each distinct geometry.

An unexpected discovery prevented utilization of the above quadratic interpolating function in this study. It is described here only because it may be of interest to other researchers, and because it explains why the more complicated cubic fit over a triangle eventually had to be used.

For reasons to be discussed in chapter 4, it would be extremely inconvenient to construct a finite element mesh for the transport equation without the use of right triangles. In the case of a right triangle the derivatives of natural coordinates with respect to  $x$  (and  $u$ ) are constrained so that two are of equal magnitude but opposite sign, and the third is identically zero. In this case  $\underline{B}$  of equation (2-21) is singular, and the right triangle is in every instance pathological for a quadratic interpolant that uses 3 fluxes and 3 derivatives as degrees of freedom.

Used instead was another quadratic interpolant, that uses values of flux at nodes and boundary centers to represent six degrees of freedom. In this case

$$\varphi = [\varphi_1 \quad \varphi_2 \quad \varphi_3 \quad \varphi_4 \quad \varphi_5 \quad \varphi_6] \quad (2-25)$$

Where the natural co-ordinates of nodes 4,5 and 6 are as

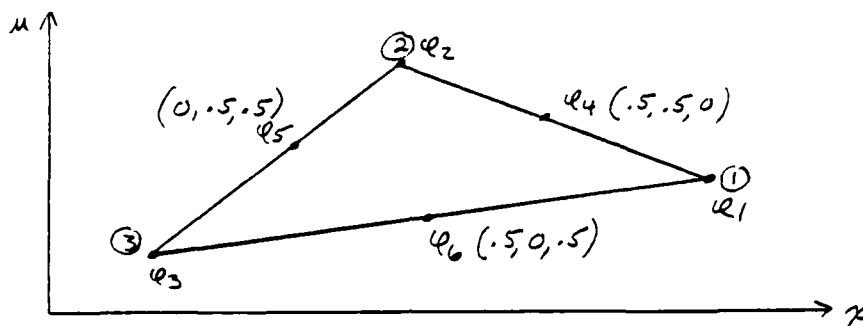


Figure 2-3  
Numbering for a  $C^0$  Quadratic Interpolant over a Triangle

given in figure 2-3. In this case  $\underline{m}$  is the same, but the matrix  $\underline{G}^T$  is no longer singular, and can now be found from the relation

$$\begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ .25 & .25 & 0 & .25 & 0 & 0 \\ 0 & .25 & .25 & 0 & .25 & 0 \\ .25 & 0 & .25 & 0 & 0 & .25 \end{bmatrix} \underline{G}^T = \underline{I} \quad (2-26)$$

and the basis functions for this interpolant are

$$\underline{h} = \underline{M} \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ -1 & -1 & 0 & 4 & 0 & 0 \\ 0 & -1 & -1 & 0 & 4 & 0 \\ -1 & 0 & -1 & 0 & 0 & 4 \end{bmatrix} \quad (2-27)$$

The cubic fit over a triangle requires that 10 degrees of freedom be specified. Chosen were flux values, and both partial derivatives at corner nodes, as well as the triangle centroid field variable value. Assigning numbers to the degrees of freedom as per below simplifies notation.

$$\begin{aligned}\hat{\underline{\phi}} &= [\phi_1 \quad \phi_{1x} \quad \phi_{1u} \quad \phi_2 \quad \phi_{2x} \quad \phi_{2u} \quad \phi_3 \quad \phi_{3x} \quad \phi_{3u} \quad \phi_4] \\ &= [\psi_1 \quad \psi_2 \quad \psi_3 \quad \psi_4 \quad \psi_5 \quad \psi_6 \quad \psi_7 \quad \psi_8 \quad \psi_9 \quad \psi_{10}] \quad (2-28)\end{aligned}$$

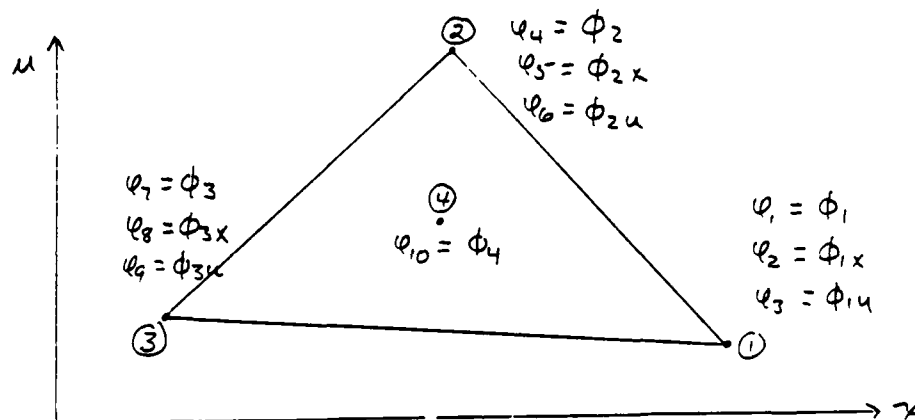


Figure 2-4  
Numbering for Cubic Fit Over a Triangle

The basis functions are again given by (2-15) except now

$$\hat{\underline{m}} = \begin{bmatrix} l_1^3 & l_1^2 l_2 & l_1^2 l_3 & l_2^3 & l_2^2 l_3 & l_2^2 l_1 & l_3^3 \\ l_3^2 l_1 & l_3^2 l_2 & l_1 l_2 l_3 \end{bmatrix} \quad (2-29)$$

$$\hat{\underline{m}}_1 = \begin{bmatrix} 3l_1^2 g_1 & 2l_1 l_2 g_1 - l_1^2 g_2 & 2l_1 l_3 g_1 + l_1^2 g_3 & 3l_2^2 g_2 \\ 2l_1 l_3 g_2 + l_2^2 g_3 & 2l_2 l_1 g_2 + l_2^2 g_1 & 3l_3^2 g_3 & 2l_3 l_1 g_3 + l_3^2 g_1 \\ 2l_3 l_2 g_3 + l_3^2 g_2 & 3l_1 l_3 + 3l_2 l_3 + 3l_3 l_1 & & \end{bmatrix} \quad (2-30)$$

$$\hat{\underline{m}}_u = \begin{bmatrix} 3l_1^2 F_1 & 2l_1 l_2 F_1 + l_1^2 F_2 & 2l_1 l_3 F_1 + l_1^2 F_3 & 3l_2^2 F_2 \\ 2l_3 l_1 F_3 + l_2^2 F_3 & 2l_2 l_1 F_2 + l_2^2 F_1 & 3l_3^2 F_3 & 2l_3 l_1 F_3 + l_3^2 F_1 \\ 2l_3 l_2 F_3 + l_3^2 F_2 & F_1 l_2 l_3 + F_2 l_1 l_3 + F_3 l_1 l_2 & & \end{bmatrix} \quad (2-31)$$

Evaluating this model at each of the 10 nodes yields the expression for  $\underline{G}_T$

$$\underline{G}_T = \underline{I} \quad (2-32)$$

$$\begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 3g_1 & g_2 & g_3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 3F_1 & F_2 & F_3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 3g_2 & g_3 & g_1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 3F_2 & F_3 & F_1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 3g_3 & g_1 & g_2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 3F_3 & F_1 & F_2 & 0 \\ \frac{1}{27} & \frac{1}{27} & \frac{1}{27} & \frac{1}{27} & \frac{1}{27} & \frac{1}{27} & \frac{1}{27} & \frac{1}{27} & \frac{1}{27} & \frac{1}{27} \end{bmatrix}$$

It is not necessary to invert the 10 x 10 matrix above if it is partitioned into 9 3 x 3 matrices and several 3 x 1 vectors as below

$$\underline{G}_T = \underline{I} \quad (2-33)$$

$$\begin{bmatrix} \underline{A} & \underline{B} & \underline{C} & \underline{D} \\ \underline{B}^T & \underline{E} & \underline{F} & \underline{G} \\ \underline{C}^T & \underline{F}^T & \underline{H} & \underline{I} \\ \underline{D}^T & \underline{G}^T & \underline{I}^T & \underline{J} \end{bmatrix}$$

if  $\tilde{S} = \begin{bmatrix} 1/27 & 1/27 & 1/27 \end{bmatrix}$  and  $\underline{G}$  is partitioned similarly then

$$\underline{G}^T = \begin{bmatrix} \underline{D} & \underline{0} & \underline{0} & \underline{0} \\ \underline{0} & \underline{E} & \underline{0} & \underline{0} \\ \underline{0} & \underline{0} & \underline{F} & \underline{0} \\ \underline{P} & \underline{Q} & \underline{R} & \underline{27} \end{bmatrix} \quad (2-34)$$

with

$$\begin{aligned} \underline{D} &= \underline{A}^{-1} & \underline{P} &= -27 \tilde{S} \underline{D} \\ \underline{E} &= \underline{B}^{-1} & \underline{Q} &= -27 \tilde{S} \underline{E} \\ \underline{F} &= \underline{C}^{-1} & \underline{R} &= -27 \tilde{S} \underline{F} \end{aligned} \quad (2-35)$$

The chore of inverting a 10 X 10 matrix is simplified. The basis functions, and the degrees of freedom for this cubic fit are specified. <sup>1</sup> C continuity is achieved with this fit. The only drawback is that the basis functions depend upon triangle geometry, and therefor must be recomputed for each unique triangle configuration.

### C. The Tetrahedron and Three Dimensional Interpolation Functions

In three dimensions the simplest element is the four node tetrahedron. Four volume coordinates,  $(L_1, L_2, L_3, L_4)$  can be used to describe this element. A straight-forward linear relation exists between x,u,u' co-ordinates and a tetrahedron's natural coordinates:

$$\begin{bmatrix} 1 & 1 & 1 & 1 \\ \eta_1 & \eta_2 & \eta_3 & \eta_4 \\ \mu_1 & \mu_2 & \mu_3 & \mu_4 \\ \mu'_1 & \mu'_2 & \mu'_3 & \mu'_4 \end{bmatrix} \begin{bmatrix} L_1 \\ L_2 \\ L_3 \\ L_4 \end{bmatrix} = \begin{bmatrix} 1 \\ \eta \\ \mu \\ \mu' \end{bmatrix} \quad (2-36)$$

(2-36) holds in a right handed system, if nodes are numbered such that nodes 1,2 and 3 progress counterclockwise when viewed from node 4.

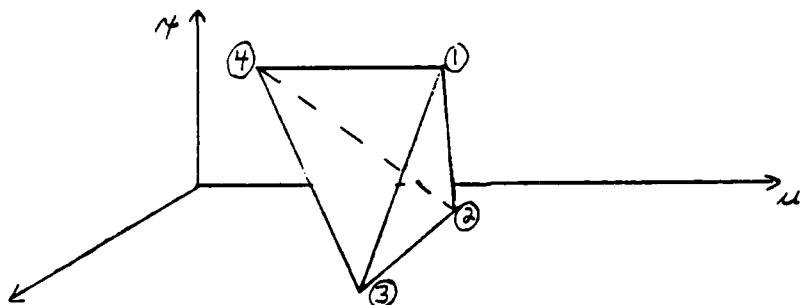


Figure 2-5  
Four Node Tetrahedron Numbering in a  
Right Handed Co-ordinate System

The partial derivatives of natural co-ordinates with respect to the  $x, y, z$  spatial variables will be needed in the next section to derive interpolating functions. If (2-36) is re-written as

$$A \begin{bmatrix} L_1 \\ L_2 \\ L_3 \\ L_4 \end{bmatrix} = \begin{bmatrix} 1 \\ \eta \\ \mu \\ \mu' \end{bmatrix} \quad (2-37)$$

and the equation is differentiated with respect to  $x$ , then

$$\begin{bmatrix} \frac{\partial L_1}{\partial x} \\ \frac{\partial L_2}{\partial x} \\ \frac{\partial L_3}{\partial x} \\ \frac{\partial L_4}{\partial x} \end{bmatrix} = \underline{\underline{A}}^{-1} \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix} \quad (2-38)$$

and the  $\frac{\partial L_i}{\partial x}$  are the second column of  $\underline{\underline{A}}^{-1}$ . Similarly  $\frac{\partial L_i}{\partial u}$  and  $\frac{\partial L_i}{\partial u'}$  are the third and fourth columns of  $\underline{\underline{A}}^{-1}$  respectively.

Integration of tetrahedral coordinates over a volume is conveniently given by (3: 148)

$$\int dV L_1^p L_2^q L_3^r L_4^s = 6V \frac{p! q! r! s!}{(p+q+r+s+3)!} \quad (2-39)$$

where V is the element volume given by

$$6V = \begin{vmatrix} 1 & 1 & 1 & 1 \\ \kappa_1 & \kappa_2 & \kappa_3 & \kappa_4 \\ \mu_1 & \mu_2 & \mu_3 & \mu_4 \\ \mu'_1 & \mu'_2 & \mu'_3 & \mu'_4 \end{vmatrix} \quad (2-40)$$

To prescribe a linear fit over this element 4 degrees of freedom must be specified. These can be the values of the flux at corner nodes so that

$$\phi = \sum_{i=1}^4 L_i \psi_i \quad (2-41)$$

A cubic requires twenty degrees of freedom in three dimensions. These can be nodal values of the flux, and the three directional derivatives at each node as well as face centered values of the flux, as per figure 2-6, with F as the

field variable. Nodes 5, 6, 7, and 8 are face centered across from nodes 1, 2, 3 and 4 respectively.

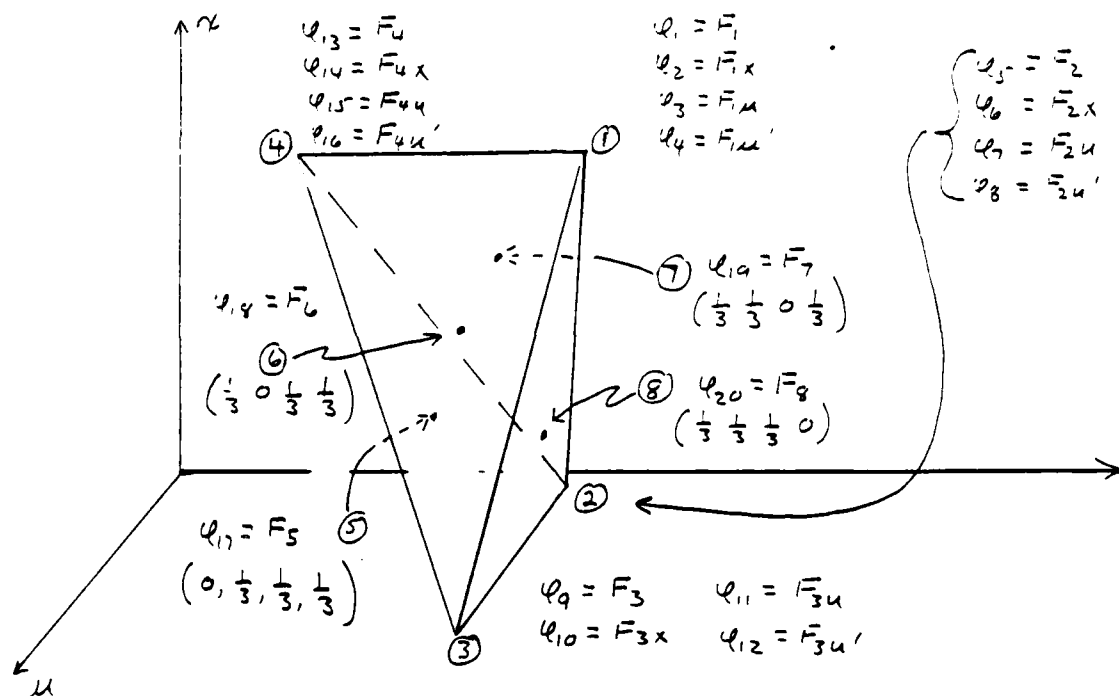


Figure 2-6  
Numbering of 20 Degrees of Freedom for a Cubic  
Fit on a 4 Node Tetrahedron

The basis functions for this fit are again given by (2-15)

with

$$\hat{m} = \begin{bmatrix} L_1^3 & L_1^2 L_2 & L_1^2 L_3 & L_1^2 L_4 & L_2^3 & L_2^2 L_1 & L_2^2 L_3 \\ L_2^2 L_4 & L_3^3 & L_3^2 L_1 & L_3^2 L_2 & L_3^2 L_4 & L_4^3 & L_4^2 L_1 \\ L_4^2 L_2 & L_4^2 L_3 & L_4 L_3 L_4 & L_1 L_3 L_4 & L_1 L_2 L_4 & L_1 L_2 L_3 \end{bmatrix} \quad (2-42)$$

G<sup>T</sup> is now a 20 X 20 matrix found by inverting

$$\begin{bmatrix}
 \underline{\underline{M1}} & \underline{\underline{0}} & \underline{\underline{0}} & \underline{\underline{0}} & \underline{\underline{0}} \\
 \underline{\underline{0}} & \underline{\underline{M2}} & \underline{\underline{0}} & \underline{\underline{0}} & \underline{\underline{0}} \\
 \underline{\underline{0}} & \underline{\underline{0}} & \underline{\underline{M3}} & \underline{\underline{0}} & \underline{\underline{0}} \\
 \underline{\underline{0}} & \underline{\underline{0}} & \underline{\underline{0}} & \underline{\underline{M4}} & \underline{\underline{0}} \\
 \underline{\underline{M5}} & \underline{\underline{M6}} & \underline{\underline{M7}} & \underline{\underline{M8}} & \underline{\underline{M9}}
 \end{bmatrix} \quad (2-43)$$

where

$$\underline{\underline{M1}} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 3e_1 & e_2 & e_3 & e_4 \\ 3f_1 & f_2 & f_3 & f_4 \\ 3g_1 & g_2 & g_3 & g_4 \end{bmatrix}$$

$$\underline{\underline{M2}} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 3e_2 & e_1 & e_3 & e_4 \\ 3f_2 & f_1 & f_3 & f_4 \\ 3g_2 & g_1 & g_3 & g_4 \end{bmatrix}$$

$$\underline{\underline{M3}} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 3e_3 & e_1 & e_2 & e_4 \\ 3f_3 & f_1 & f_2 & f_4 \\ 3g_3 & g_1 & g_2 & g_4 \end{bmatrix}$$

$$\underline{\underline{M4}} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 3e_4 & e_1 & e_2 & e_3 \\ 3f_4 & f_1 & f_2 & f_3 \\ 3g_4 & g_1 & g_2 & g_3 \end{bmatrix}$$

$$\underline{\underline{M5}} = \begin{bmatrix} 0 & 0 & 0 & 0 \\ k_{27} & 0 & k_{27} & k_{27} \\ k_{27} & k_{27} & 0 & k_{27} \\ k_{27} & k_{27} & k_{27} & 0 \end{bmatrix}$$

$$\underline{\underline{M6}} = \begin{bmatrix} k_{27} & 0 & k_{27} & \frac{1}{27} \\ 0 & 0 & 0 & 0 \\ \frac{1}{27} & \frac{1}{27} & 0 & \frac{1}{27} \\ \frac{1}{27} & \frac{1}{27} & \frac{1}{27} & 0 \end{bmatrix}$$

$$\underline{\underline{M7}} = \begin{bmatrix} \frac{1}{27} & 0 & \frac{1}{27} & \frac{1}{27} \\ \frac{1}{27} & \frac{1}{27} & 0 & \frac{1}{27} \\ 0 & 0 & 0 & 0 \\ \frac{1}{27} & \frac{1}{27} & \frac{1}{27} & 0 \end{bmatrix}$$

$$\underline{\underline{M8}} = \begin{bmatrix} \frac{1}{27} & 0 & \frac{1}{27} & \frac{1}{27} \\ \frac{1}{27} & \frac{1}{27} & 0 & \frac{1}{27} \\ \frac{1}{27} & \frac{1}{27} & \frac{1}{27} & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\underline{\underline{M9}} = \begin{bmatrix} \frac{1}{27} & 0 & 0 & 0 \\ 0 & \frac{1}{27} & 0 & 0 \\ 0 & 0 & \frac{1}{27} & 0 \\ 0 & 0 & 0 & \frac{1}{27} \end{bmatrix}$$

and  $e_1 = \frac{\partial L_1}{\partial x}$ ,  $f_1 = \frac{\partial L_1}{\partial u}$ ,  $g_1 = \frac{\partial L_1}{\partial u}$ ,

and so on. If  $\underline{\underline{G^T}}$  is partitioned into

$$\underline{\underline{G^T}} = \begin{bmatrix} \underline{\underline{M10}} & \underline{\underline{0}} & \underline{\underline{0}} & \underline{\underline{0}} & \underline{\underline{0}} \\ \underline{\underline{0}} & \underline{\underline{M11}} & \underline{\underline{0}} & \underline{\underline{0}} & \underline{\underline{0}} \\ \underline{\underline{0}} & \underline{\underline{0}} & \underline{\underline{M12}} & \underline{\underline{0}} & \underline{\underline{0}} \\ \underline{\underline{0}} & \underline{\underline{0}} & \underline{\underline{0}} & \underline{\underline{M13}} & \underline{\underline{0}} \\ \underline{\underline{M14}} & \underline{\underline{M15}} & \underline{\underline{M16}} & \underline{\underline{M17}} & \underline{\underline{M18}} \end{bmatrix}$$

(2-44)

then

$$\underline{M}_{10} = \underline{M}_1^{-1} \quad (2-45)$$

$$\underline{M}_{11} = \underline{M}_2^{-1} \quad (2-46)$$

$$\underline{M}_{12} = \underline{M}_3^{-1} \quad (2-47)$$

$$\underline{M}_{13} = \underline{M}_4^{-1} \quad (2-48)$$

$$\underline{M}_{18} = 27 \underline{I} \quad (2-49)$$

$$\underline{M}_{14} = -\underline{M}_{18} \underline{M}_5 \underline{M}_{10} \quad (2-50)$$

$$\underline{M}_{15} = -\underline{M}_{18} \underline{M}_6 \underline{M}_{11} \quad (2-51)$$

$$\underline{M}_{16} = -\underline{M}_{18} \underline{M}_7 \underline{M}_{12} \quad (2-52)$$

and

$$\underline{M}_{17} = -\underline{M}_{18} \underline{M}_8 \underline{M}_{13} \quad (2-53)$$

The basis functions for this fit are defined. They depend upon element geometry, and require that 4 separate 4 X 4 matrices be inverted.

### C. Summary

This study uses two elements to construct finite element meshes. They are the triangle and the four node tetrahedon. Describing these elements in terms of their natural coordinates is straightfoward, and will be seen to simplify later calculations.

Four interpolating functions, one linear, two quadratic and one cubic were investigated over a triangle. The quadratic that uses partial derivatives as degrees of freedom turns out to be singular for right triangles, so a quadratic <sup>0</sup>C fit was substituted. Two fits were done on the

tetrahedron, a linear and a cubic. Any fit that uses field variable derivatives as interpolants has geometry dependent basis functions. These increase the number of calculations required since they must be found for each distinct element geometry.

### 3. The Case of no Scatter

With scattering cross section of zero, the expression to be digitized (1-16) becomes

$$I = \frac{1}{2} \int dx du u^2 \left( \frac{\partial \phi}{\partial x} \right)^2 + \frac{1}{2} \int dx du \Sigma_t \phi^2 - \frac{1}{2} \int dx du 2u \Sigma_t \phi \frac{\partial \phi}{\partial x} \quad (3-1)$$

Only particle streaming and absorption is occurring. The first integral of (3-1) is referred to as the streaming term, since it represents particle streaming, the second term is called the absorbing term for the analogous reason, and the third term is the boundary term. This last integral results from the cross product of streaming and absorbing terms and is referred to as the boundary contribution since without it the natural boundary conditions which arise from the integration by parts in equation (1-12) are not satisfied. These three terms are referred to as local since they fit field variable values limited to the triangle under scrutiny. In this section, a description of these terms' derivation and preparation for digitization will occur. Since the quadratic and cubic fits involve extremely long derivations, their results only are presented in appendices. Lastly, a test case to which an analytical solution exists is described, and numerical results of the various fits' digitization are presented.

#### A. The Local Terms

1. The Absorbing Term. Recalling (2-17) the interpolating function for  $\phi$

$$\phi = \underline{\hat{m}} \underline{G^T} \underline{\psi} \quad (2-17)$$

or

$$\phi = \underline{\hat{\psi}} \underline{\underline{G^T}} \underline{m} \quad (3-1)$$

$$\int_{\Delta_i} \phi_i = \frac{\bar{\mu}_i - \mu_i}{6} \tilde{\phi}_i \underline{G}_i^T \left[ \underline{m}(\underline{l}_1, \underline{l}_2, \underline{l}_3) + \right. \\ \left. 4 * \underline{m}(\underline{l}_1, \underline{l}_2, \underline{l}_3) + \underline{m}(\underline{l}_1, \underline{l}_2, \underline{l}_3) \right] \quad (4-11)$$

$$= \tilde{\phi}_i \underline{LI} x = c \quad (4-12)$$

Since the integration over X involves 3 points, LI ( local integral ) (of dimension 10x1) and NLI (of dimension 1x10) must be evaluated at x=a, b and c, then

$$\underline{NLM}(i, j, k, l) = \left( \frac{a-c}{6} \right) * \tilde{\phi}_i \left[ \underline{LI}_a \underline{NLI}_a + \right. \\ \left. 4.0 * \underline{LI}_b \underline{NLI}_b + \underline{LI}_c \underline{NLI}_c \right] \phi_j \quad (4-13)$$

where NLM is the (10 X 10) (k x l) non local matrix reflecting triangle i scattering to triangle j. The five triangle column produces 25 such non local matrices, all of which must be assembled globally, and must be saved if triangle penalties are desired as mesh refinement indicators.

In appendix G, subroutine LCORD finds the natural coordinates of the points (49 for Weddle's n=6) needed on each triangle for integration, and evaluates  $\underline{m}$  and  $\underline{m}_\gamma$  (needed to evaluate the second scattering integral) at each of these points. ANING performs the angle integrals, finding matrices  $\underline{LI}$  and  $\underline{NLI}$ . Finally SPING calculates the space integral across the width of the triangle. The subroutines are well documented, with a list

Simpson's method yields

$$\int_{u \in \Delta_j} du' \phi(x, u') \approx \frac{(\bar{u}_j - \underline{u}_j)}{6} \left[ \phi(x, \underline{u}_j) + 4 * \phi(x, \bar{u}_j) + \phi(x, \bar{u}_j) \right] \quad (4-8)$$

where  $\bar{u}_j = u$  of triangle  $j$ , upper ( $x$  fixed)  
 $\underline{u}_j = u$  of triangle  $j$ , middle  
 $\underline{u}_j = u$  of triangle  $j$ , lower

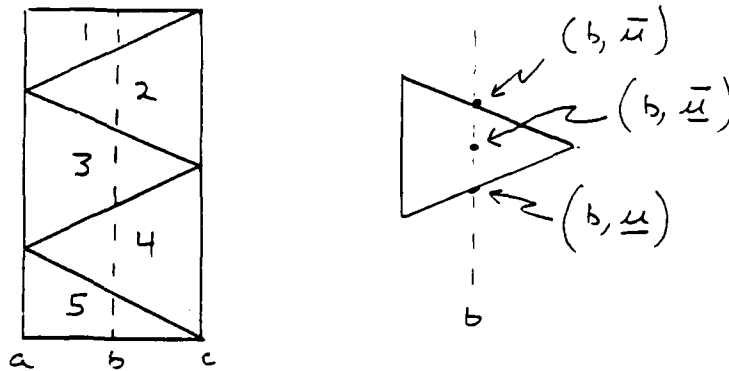


Figure 4-3

Sample 5 triangle column with U upper, lower and center of triangle 3 for  $X = B$

which, in terms of the interpolation functions is

$$= \left( \frac{\bar{u}_j - \underline{u}_j}{6} \right) \left[ \tilde{m}(\underline{l}, \underline{l}_2, \underline{l}_3) + 4 * \tilde{m}(\underline{l}, \bar{l}_2, \underline{l}_3) + \tilde{m}(\underline{l}, \bar{l}_2, \bar{l}_3) \right] * \underline{G}_j \underline{\psi}_j' \quad (4-9)$$

$$= \underline{NL I}_{x=c} \underline{\psi}_j' \quad (4-10)$$

where  $\tilde{m}(\underline{l}, \underline{l}_2, \underline{l}_3)$  represents  $\tilde{m}$  evaluated at the natural coordinates of  $(c, \bar{u}_j)$  referred to as  $(\underline{l}, \bar{l}_2, \bar{l}_3)$ , and  $\underline{NL I}_{x=c}$  is the non local integral of triangle  $j$  at  $x = c$ .

Similarly, over the local triangle

triangles, was abandoned.

### C. Numerical Evaluation of the Scattering Integrals

The first attempt to evaluate the scattering terms was to calculate the integrals with numerical approximations. Since the cubic fit provides such high accuracy, it was felt that the very good streaming and absorbing approximations, with less accurate scattering, would provide solutions properly reflecting the physics involved in a problem.

Simpson's rule integration, Weddle's, and Weddle's rule for  $n=6$  were sequentially tried. This section will describe Simpson's integration for one of the scattering terms, since it is the simplest to write out. The second integral and the other two techniques are straightforward extensions, and appendix H contains subroutines used numerically to evaluate both scattering integrals with Weddle's rule for  $n=6$ .

In the case of integral A

$$\int_a^c dx \int_{-1}^1 du \int_{-1}^1 du' \propto \phi \phi' \quad (4-6)$$

where  $\propto = (\frac{\xi_s^2}{2} - \xi_s \xi_t)$ , summation over the 5 triangle column of figure 4-3, is represented as

$$= \propto \int_a^c dx \sum_{i=1}^5 \int_{u \in \Delta_i} du \phi(x, u) \sum_{j=1}^5 \int_{u' \in \Delta_j} du' \phi(x, u') \quad (4-7)$$

where  $u \in \Delta_i$  represents integration over  $u$  in triangle  $i$ .

problem to simplify evaluation of the integral in this manner.

If meshes are constrained columnarly as in figure 4-2, then for example, integral A is

$$\begin{aligned} & \left( \frac{\xi_s^2}{2} - \xi_s \xi_t \right) \int_a^b dx \int_{-1}^1 \int_{-1}^1 du du' \phi \phi' \\ & = \left( \frac{\xi_s^2}{2} - \xi_s \xi_t \right) \int_a^b dx \int_{-1}^1 \int_{-1}^1 du du' \sum_{i=1}^n \sum_{j=1}^n \phi_i \phi_j' \end{aligned} \quad (4-5)$$

where n is the number of triangles in a column. Integration over u, can proceed from the column's top triangle to the

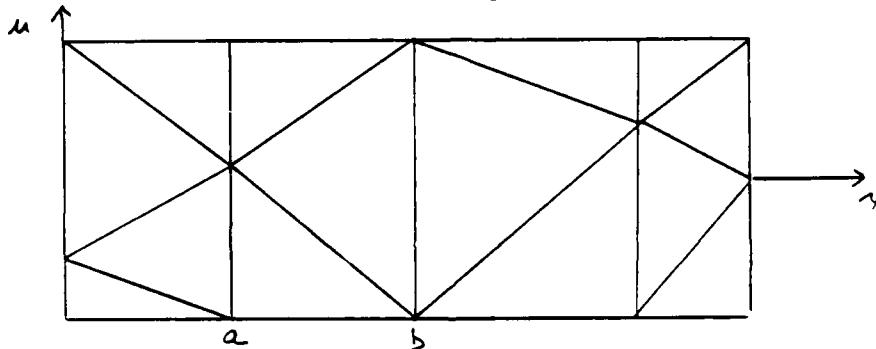


Figure 4-2  
Columnar Finite Element Mesh

bottom triangle, one element at a time, halting at each triangle to integrate over u' for all elements in a column. Since n is the number of triangles in a column, n\*n angle integrals are evaluated per column. Each integral is integrated over space separately and results in a non local matrix that must be assembled globally. The bookkeeping involved in evaluating the two scattering integrals is simplified. For this reason, the quadratic fit using derivatives as finite element nodes discussed in chapter 2, found to be nonexistent in right

these terms numerically, and with analytical approximations, and describes the results of these efforts. The cubic interpolant of chapter 3 was used as the finite element approximation for flux.

#### B. Mesh Arrangement

Integration of equation (4-3) is over both angular variables  $u$  and  $u'$ . This proves to be cumbersome. Consider integration from  $x=a$  to  $x=b$  of Figure 4-1

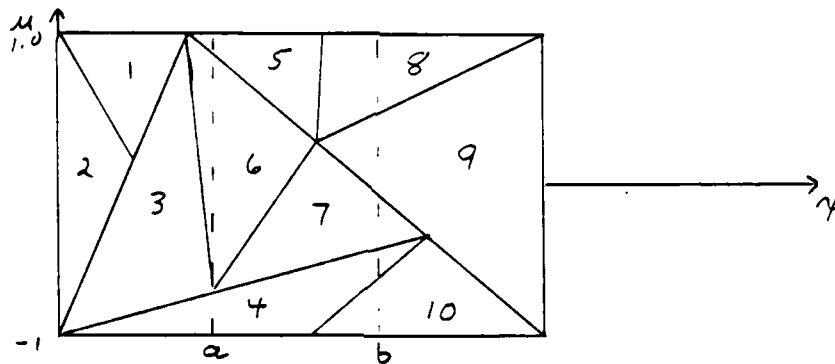


Figure 4-1  
An Unrestricted Finite Element Mesh  
Over the Benchmark Solution Domain of  
Figure 3-1

$$\int_a^b \int_{-1}^1 \int_{-1}^1 du' du dx \quad (4-4)$$

$\phi$  and  $\phi_x$  are given by differing cubic interpolation functions in each of the 7 triangles composing this area. Proper bookkeeping becomes a serious challenge.

To avoid this, triangles are restricted to columns. While this makes successive mesh refinement cumbersome, and will probably be awkward if the method is ever extended to another dimension, it is certainly appropriate for an early cut at the

#### 4. The Case of Isotropic Scatter

##### A) The Non Local Terms

When Scattering is allowed to occur (1-16) must be evaluated in its entirety. This equation can be rewritten as

$$\frac{1}{2} \iiint dx du \left\{ \mu^2 \left( \frac{\partial \phi}{\partial x} \right)^2 + \Sigma_z^2 \phi^2 + 2\mu \Sigma_z \frac{\partial \phi}{\partial x} \phi + \left( -\mu \Sigma_s \frac{\partial \phi}{\partial x} - \Sigma_z \Sigma_s \phi \right) \int_{-1}^1 du' \phi' + \frac{\Sigma_s}{2} \int_{-1}^1 du' \phi' \frac{\Sigma_s}{2} \int_{-1}^1 du'' \phi'' \right\} \quad (4-1)$$

If one neglects the three local integrals the non local, or scattering integrals are left,

$$\frac{1}{2} \iiint dx du du' \frac{\Sigma_s^2}{4} \phi' \int_{-1}^1 \phi'' du'' + \frac{1}{2} \iiint dx du du' \left( -\mu \Sigma_s \frac{\partial \phi}{\partial x} - \Sigma_z \Sigma_s \phi \right) \phi' \quad (4-2)$$

Since there is no u dependence in the first integral, it may be integrated out, then a change of variables from u'' to u may occur, allowing both integrals to be combined, resulting in

$$\frac{1}{2} \iiint dx du du' \left( \frac{\Sigma_s^2}{2} - \Sigma_z \Sigma_s \right) \phi \phi' + \frac{1}{2} \iiint dx du du' \left( -\mu \Sigma_s \right) \frac{\partial \phi}{\partial x} \phi' \quad (4-3)$$

These are the two scattering integrals. Since they involve integration over u and u', they result in non-local terms. Only one of them ( $\phi \phi'$ ) results in a naturally symmetric non-local matrix after global assemblage. These integrals are referred to as A and B in this report and the code of appendix A. This section describes the preparation for digitization of

mesh 4 is worse than meshes 2 and 3. Scrutiny of element penalties reveals that this is due to elements of mesh 4 being refined at the area where the largest derivative discontinuity occurs (  $x=0$ , elements 4 and 5 ). This can be considered as

Mesh	Total Penalty		
	linear	quadratic	cubic
1	.02556	.00337	.000398
2	.01074	.000559	.0000474
3	.01433	.000637	.0000526
4	.00716	.000373	.0000502
5	.00136	.000067	.0000158
6	.00101		

Table 3-3  
Mesh Penalties as Convergence Indicators

further evidence of the cubic fits' power, it is flagging to the programmers attention the nonphysical boundary condition; the  $C^0$  fits are not sophisticated enough to display the anomaly.

#### E. Summary

The three terms which comprise the transport functional in the case of no scatter are all local. Their derivations are straightforward and nearly trivial in the linear case. For higher order interpolants the derivation is still easy to follow, but very long. When assembled globally these terms represent the transport functional. Setting the variation of this functional to zero leaves a positive definite set of simultaneous linear equations that is solved to find nodal values. The cubic interpolant (with  $C^1$  continuity) is more powerful, and may be faster than the  $C^0$  interpolants, which require excessive mesh refinement before converging. Penalties are powerful indicators of convergence.

Two pieces of data appear as anomalies in Table 3-2. The first of these is that the cubic fit for mesh 1 appears better than mesh 2 or 3. Table 3-3 lists total penalties of the meshes, and indicates that since mesh 2 and mesh 3 have lower penalties, the finite element fit is actually better in these meshes. Mesh 1 was "lucky" for the cubic in that nodal values came out so close to the analytical.

For $u > 0$		Avg Perc Diff of Analytic to Numeric			
Mesh	# of Triangles / Mean Free Path	Linear      Quadratic      Cubic			
1	1.33	46.6 (1.5)	13.73 (4.1)	1.37 (9.2)	
2	2.00	28.4 (2.2)	5.55 (5.5)	2.83 (12.1)	
3	2.00	29.5 (2.3)	5.64 (6.7)	2.76 (12.1)	
4	3.67	27.2 (2.9)	4.24 (8.5)	.84 (18.8)	
5	8.50	8.7 (5.0)	5.45 (17.4)	.55 (35.2)	
6	21.33	3.3 (14.3)	... ..	... ..	

Table 3-2  
Comparison of Mesh Refinement Required For Convergence of Local Terms. Average Percent Difference is From Analytic to Numerical Solution for  $u > 0$ . Values in Parenthesis are CPU Seconds of Runtime on a Vax 11-780, unix Berkely 1.2, During Periods of Moderate to Almost Heavy Use.

Likewise mesh 5 for the quadratic fit appears worse than less refined meshes. The total penalty bears out that mesh 5 is a better fit. These and other similar experiences emphasis two points that should not be neglected with the finite element method. The first of these is that element penalties can be as good a measure of convergence, or better, than comparing nodal values to some "exact" solution. Secondly, the meshes used in this study are not necessarily successively refined. Without this type of refinement, steady convergence of nodal values to the exact solution may not be observed (3:79).

One anomaly appears in table 3-3. That is the cubic fit for

refinement. The difference is clearly caused because flux

u=1	x	Analytic	Linear	Quadratic	Cubic
	.375	.6873	.6360	.6904	.6865
	1.000	.4724	.3834	.4282	.4707
	1.500	.2231	.1405	.1707	.2230
	3.000	.0498	.0270	.0302	.0512
CPU units (sec's)	...		2.9	8.5	18.8

Table 3-1  
Comparison for Mesh 4 of Accuracy  
and Run Times for 3 Interpolation Fits on a Vax 11-780  
(unix, Berkely 1-2) for u=1

spatial derivatives are held continuous in the  $C^1$  fit. The  $C^0$  quadratic fit is only slightly better than the linear. Consider the expansion of 1-17 and 1-18 in the no scattering case.

$$-2\mu^2 \frac{\partial^2 \phi}{\partial x^2} + 2\varepsilon_t^2 \phi = 0 \quad (1-17a)$$

$$2\mu \left[ \mu \frac{\partial \phi}{\partial x} + \varepsilon_t \phi \right] = 0 \quad (1-18a)$$

These are the differential equations being satisfied when the variational functional is minimized, and the natural boundary condition. Three quantities in these equations must be approximated by finite elements,  $\phi$ ,  $\frac{\partial \phi}{\partial x}$  and  $\frac{\partial^2 \phi}{\partial x^2}$ .  $C^0$  continuity holds only one of these continuous across elements boundaries. The  $C^1$  fit holds two of the three continuous and as a result converges faster. This analysis further indicates that a  $C^2$  fit would converge even faster, and a  $C^3$  fit would be no better than a  $C^2$ , since no higher order terms are needed to satisfy these equations.

$$\phi = u \geq \frac{-\epsilon_+ u}{u} \quad u > 0 \quad (3-19)$$

$$\text{and} \quad \phi = 0 \quad u \leq 0 \quad (3-20)$$

Since most streaming is occurring near  $u = 1$ , meshes were refined more in that area. Also, notice that the boundary conditions are not physical, there is a discontinuity of derivatives along the  $u=0$  line. For now one must realize that this discontinuity is a source of error that becomes apparent for  $u$  near zero.

### C. Results

The area of the Benchmark problem was discretized with 6 separate meshes for the computer runs. All are drawn and listed in appendix F. Meshes 1 through 5 are those used by Goff (2:114) while mesh 6 is a very well refined mesh of 80 triangles in 3 mean free paths. Mesh 2 and 3 consist of the same number of triangles, but with a different pattern, to test sensitivity to element orientation. Table 3-1 shows a comparison of interpolation fit accuracy with the analytical solution for mesh 4.

Table 3-2 Lists the average nodal percent difference from the analytical solution to allow a comparison of the degree of mesh refinement required for convergence. It is seen from these results that the cubic fit is extremely powerful. Run times should not be taken as absolute, but it appears that the price paid in terms of extra calculations for the more accurate fit is not extreme. The linear fit converges as finite element theory says it will, but only with an excessive amount of mesh

performed for a triangle, the resultant quadratic form can be written as

$$I = \frac{1}{2} \hat{\phi}^T \hat{\phi}^T \left[ \underline{\underline{M}}_A + \underline{\underline{M}}_B + \underline{\underline{M}}_S \right] \underline{\underline{G}}^T \underline{\underline{\phi}} = \frac{1}{2} \hat{\phi}^T \underline{\underline{G}}^T \underline{\underline{M}}_L \underline{\underline{G}}^T \underline{\underline{\phi}} \quad (3-17)$$

where  $\underline{\underline{M}}_L$  is the local matrix. The global assemblage of these local matrices results in a quadratic form for the variational integral over the entire area under scrutiny. When minimized, the remaining set of simultaneous linear equations has a coefficient matrix that is always positive definite, and is solved by cholesky decomposition in this study.

#### B. The Test Case

The problem chosen to test the digitization of the local terms was a monoenergetic lambertian (flux = cosine of the angle it is traveling) source of particles incident upon an absorbing only slab 3 mean free paths thick. The slab is surrounded on both sides by a vacuum so there is no returning flux from the right boundary.

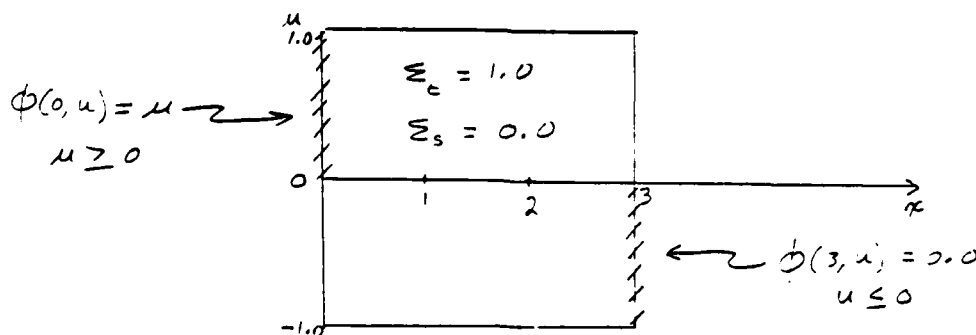


Figure 3-1  
Benchmark Problem Description

In this case the transport equation is

$$\mu \frac{\partial \phi}{\partial x} + \Sigma_c \phi = 0 \quad (3-18)$$

The solution is

interpolant evaluation are in appendix C .

### 3. The Streaming term.

Expansion of  $u$  yields six integrals which must be evaluated.

$$u^2 = u_1^2 l_1^2 + u_2^2 l_2^2 + u_3^2 l_3^2 + 2u_1 u_2 l_1 l_2 + 2u_1 u_3 l_1 l_3 + 2u_2 u_3 l_2 l_3 \quad (3-11)$$

$$\begin{aligned} \frac{1}{2} \int dA u^2 \left( \frac{\partial \Phi}{\partial x} \right)^2 &= \frac{1}{2} \hat{\underline{Q}} \hat{\underline{G}}^T \left[ \int dA u_1^2 l_1^2 \underline{m}_x \hat{\underline{m}}_x + \int dA u_2^2 l_2^2 \underline{m}_x \hat{\underline{m}}_x \right. \\ &+ \int dA u_3^2 l_3^2 \underline{m}_x \hat{\underline{m}}_x + \int dA 2u_1 u_2 l_1 l_2 \underline{m}_x \hat{\underline{m}}_x \\ &+ \left. \int dA 2u_1 u_3 l_1 l_3 \underline{m}_x \hat{\underline{m}}_x + \int dA 2u_2 u_3 l_2 l_3 \underline{m}_x \hat{\underline{m}}_x \right] \hat{\underline{G}}^T \underline{Q} \quad (3-12) \end{aligned}$$

$$= \frac{1}{2} \hat{\underline{Q}} \hat{\underline{G}}^T \left[ \underline{MS1} + \underline{MS2} + \underline{MS3} + \underline{MS4} + \underline{MS5} + \underline{MS6} \right] \hat{\underline{G}}^T \underline{Q} \quad (3-13)$$

$$= \frac{1}{2} \hat{\underline{Q}} \hat{\underline{G}}^T \underline{MS} \hat{\underline{G}}^T \underline{Q} \quad (3-14)$$

When linear interpolants are substituted the streaming term is

$$\underline{MS} = \frac{F}{24A} \begin{bmatrix} g_1^2 & g_1 g_2 & g_1 g_3 \\ g_1 g_2 & g_2^2 & g_2 g_3 \\ g_1 g_3 & g_2 g_3 & g_3^2 \end{bmatrix} \quad (3-15)$$

where  $F = u_1(u_1 + u_2) + u_2(u_2 + u_3) + u_3(u_3 + u_1) \quad (3-16)$

Derivation of this term for the quadratic and cubic fits are the most lengthy of all; results of this effort are in appendix D.

4. The Local Matrix. The sum of these three terms, evaluated over a triangle in the mesh, is the value of the variational integral over that element. After these calculations are

The Boundary term can be written as

$$\frac{1}{2} \int dA \varepsilon_{\pm} 2\mu \frac{\partial \phi}{\partial x} \phi = \varepsilon_{\pm} \int dA \mu \hat{\underline{\underline{\psi}}} \hat{\underline{\underline{G}}}^T \underline{\underline{m}}_x \hat{\underline{\underline{m}}} \underline{\underline{G}}^T \underline{\underline{\psi}} \quad (3-6)$$

using (2-17) and since

$$\frac{\partial \phi}{\partial x} = \frac{\partial}{\partial x} \left[ \hat{\underline{\underline{\psi}}} \hat{\underline{\underline{G}}}^T \underline{\underline{m}} \right] = \hat{\underline{\underline{\psi}}} \hat{\underline{\underline{G}}}^T \underline{\underline{m}}_x \quad (3-7)$$

the Boundary term can be expressed as the sum of three integrals

$$= \sum_{i=1}^3 \varepsilon_{\pm} \int dA \mu_i \hat{\underline{\underline{\psi}}} \hat{\underline{\underline{G}}}^T \underline{\underline{m}}_x \hat{\underline{\underline{m}}} \underline{\underline{G}}^T \underline{\underline{\psi}} \quad (3-8)$$

in the linear case, evaluation of the integral yields

$$= \frac{1}{2} \hat{\underline{\underline{\psi}}} \hat{\underline{\underline{G}}}^T \left[ \mu_1 \varepsilon_{\pm} 2A \begin{bmatrix} 2g_1 & g_2 & g_3 \\ 2g_1 & g_2 & g_3 \\ 2g_1 & g_2 & g_3 \end{bmatrix} + \mu_2 \varepsilon_{\pm} 2A \begin{bmatrix} g_1 & 2g_2 & g_3 \\ g_1 & 2g_2 & g_3 \\ g_1 & 2g_2 & g_3 \end{bmatrix} + \mu_3 \varepsilon_{\pm} 2A \begin{bmatrix} g_1 & g_2 & 2g_3 \\ g_1 & g_2 & 2g_3 \\ g_1 & g_2 & 2g_3 \end{bmatrix} \right] \underline{\underline{G}}^T \underline{\underline{\psi}}$$

$$= \frac{1}{2} \hat{\underline{\underline{\psi}}} \hat{\underline{\underline{G}}}^T \left[ \underline{\underline{MB1}} + \underline{\underline{MB2}} + \underline{\underline{MB3}} \right] \underline{\underline{G}}^T \underline{\underline{\psi}} = \frac{1}{2} \hat{\underline{\underline{\psi}}} \hat{\underline{\underline{G}}}^T \underline{\underline{MB}} \underline{\underline{G}}^T \underline{\underline{\psi}} \quad (3-9)$$

The resultant matrix will not be symmetric, but since for each quadratic form, only one symmetric matrix exists (4:342), the boundary term can be symmetrized. That is

$$\frac{1}{2} \int dA \varepsilon_{\pm} \mu \frac{\partial \phi}{\partial x} \phi = \frac{1}{2} \hat{\underline{\underline{\psi}}} \hat{\underline{\underline{G}}}^T \left[ \left( \underline{\underline{MB}} + \hat{\underline{\underline{MB}}} \right) / 2, 0 \right] \underline{\underline{G}}^T \underline{\underline{\psi}} \quad (3-10)$$

This term is much more complicated to encode than the absorbing term, since it involves derivatives of natural coordinates with respect to x, which are different for each separate geometry. The results of quadratic and cubic

The absorbing term can be written as

$$\begin{aligned} \frac{1}{2} \int dA \epsilon_t \phi^2 &= \frac{\epsilon_t^2}{2} \int dA \hat{\phi} \hat{G}^T \underline{m} \hat{m} \underline{G}^T \underline{\phi} \\ &= \frac{\epsilon_t^2}{2} \hat{\phi} \hat{G}^T \left[ \int dA \underline{m} \hat{m} \right] \underline{G}^T \underline{\phi} \end{aligned} \quad (3-2)$$

Since  $\underline{\phi}$  and  $\underline{G}^T$  are constant within an element, they can be removed from the integral. Evaluation of the term then reduces to taking the product of  $\underline{m} \hat{m}$  and analytically performing the integral.

In the linear case  $\underline{G}^T = \underline{I}$  and

$$\underline{m} \hat{m} = \begin{bmatrix} l_1 \\ l_2 \\ l_3 \end{bmatrix} \begin{bmatrix} l_1 & l_2 & l_3 \end{bmatrix} = \begin{bmatrix} l_1^2 & l_1 l_2 & l_1 l_3 \\ l_1 l_2 & l_2^2 & l_2 l_3 \\ l_1 l_3 & l_2 l_3 & l_3^2 \end{bmatrix} \quad (3-3)$$

which, using (2-7) is

$$\epsilon_t^2 \int dA \underline{m} \hat{m} = \frac{2A \epsilon_t^2}{4!} \begin{bmatrix} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2 \end{bmatrix} = \underline{MA} \quad (3-4)$$

where  $A$  is the area of the triangle.

The absorbing term can now be written as

$$\frac{1}{2} \int dA \epsilon_t^2 \phi^2 = \frac{1}{2} \hat{\phi} \left[ \hat{G}^T \underline{MA} \underline{G}^T \right] \underline{\phi} \quad (3-5)$$

It is precisely the above expression in brackets which is digitized and evaluated for each element.

With the  $C^0$  quadratic fit, and  $C^1$  cubic previously described in chapter 2, the term derivation is analagous, expect that  $\underline{MA}$  in these cases is of order 6 and 10 respectively. Appendix B has results of these computations.

## 2. The Boundary term

of variables included in the appendix.

Note that LI and NLI are actually the same integral, just over different triangles.

$$\int du \phi = \widehat{LI}$$

$$\int du' \phi' = \widehat{NLI} = \widehat{LI}$$

Subroutine ANING takes advantage of the fact that  $\widehat{LI} = \widehat{NLI}$  and calculates the  $\int du \phi$  over every triangle in the mesh, storing it in memory to be recalled when needed. Simultaneously it calculates  $\int du u \phi_x$ , the only other angle integral needed, storing these in ILFD.

#### D. Cubic Analytical Approximation

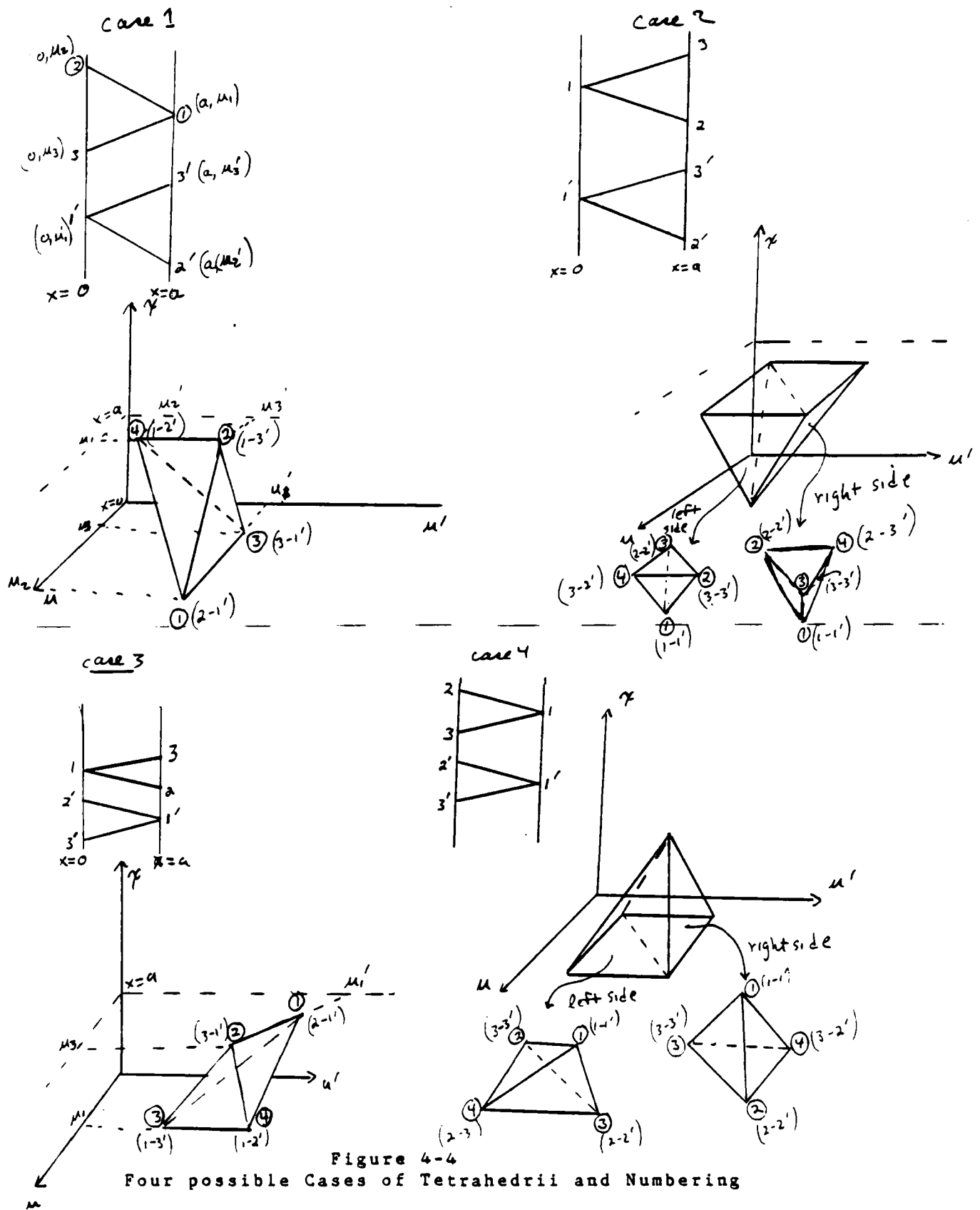
Since  $\phi$  and  $\phi_x$  are approximated with cubic functions, the scattering integrals of eqn (4-3), which integrate the products of  $\phi$  and  $\phi_x$  are integrating a hexadic. Explained in this section is an attempt to substitute another cubic for the "exact" sixth order fit required by  $\phi\phi'$  and  $\phi_x\phi'$ .

In three dimensions, the local and non local triangles map out tetrahedrons. Four possible cases can occur, depending upon the orientation of the local and non local triangles as depicted in Figure 4-4. Case 2 and case 4 result in pyramids, which can split along their center into two four node tetrahedra each, and integration can then be performed separately over each tetrahedron, and summed.

Consider the first scattering integral

$$\int dx du du' \alpha \phi \phi' \quad (4-14)$$

$$= \alpha \int dx du du' F \quad (4-15)$$



F, the product can be approximated in three dimensions with a cubic polynomial of complete basis as

$$F = \hat{\underline{m}} \underline{G}^T \underline{f} \quad (4-16)$$

where  $\underline{m}$  and  $\underline{G}^T$  are as given in (2-41) and (2-44) respectively. F can be considered to be a column matrix of twenty 10 X 10 matrices, one representing F at each of the twenty nodes of figure 2-6. For instance, case 1, node 1 is the intersection of nodes 2 (local) and node 1 (primed). f is then

$$f_1 = \phi_2 \phi_1' = \hat{\underline{\psi}} \underline{\underline{G}}^T \underline{m} \hat{\underline{m}}' \underline{\underline{G}}^T' \underline{\psi}' \quad (4-17)$$

evaluation of  $\underline{m}$  at (0,1,0) and  $\hat{\underline{m}}'$  at (1,0,0), and carrying out the multiplication is guaranteed to yield

$$f_1 = \hat{\underline{\psi}} \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \quad (4-18)$$

since both  $\phi_2$  and  $\phi_1'$  are finite element interpolation nodes.

With this cubic approximation, the second scattering integral is only slightly more complicated.

$$-\Sigma_S \int d^3x du du' u \phi_x \phi' = -\Sigma_S \int d^3x du du' (u_1 L_1 + u_2 L_2 + u_3 L_3 + u_4 L_4) G \quad (4-19)$$

if the same cubic approximation is made for  $G = \phi_x \phi'$

$$G = \hat{\underline{m}} \underline{\underline{G}}^T \underline{a} \quad (4-20)$$

then four integrals, caused by the expansion of  $u$ , must be evaluated.

The  $f_i$ 's and  $g_i$ 's are in most instances trivial, and can be written down by inspection for each of the four cases. This is done in appendix E.

The integrations are simple compared to those done for the streaming case since there are no cross products of  $\underline{m}$  and  $\underline{m}_x$ .

#### E. The Test Case

Chosen to test the numerical and analytical evaluations of the integrals was the same domain as in the no scattering case, with the region depth under scrutiny varying from one to five mean free paths. Graciously provided by Dr. Shankland was a spherical harmonics solution of the problem using up to 46 legendre polynomials. Results of these calculations are listed in appendix G for scattering cross sections corresponding to  $c$  of .5 and .9 where  $c\Sigma_t = \Sigma_s$ . Dr. Shankland used as a lower right boundary condition no return flux at infinity. Therefore, the lower right boundary used in the finite element solution is the  $P_n$  angular flux for  $u < 0$  at 1,2,3,4 or 5 mean free paths, depending upon the depth of investigation desired. In this case, there are no sources in the region under scrutiny, and the coupled  $P_n$  equations are solved with a Green's function.

The lambertian source, depicted in figure 3-1 is non physical. The derivative discontinuity at  $x=0$  is very difficult to approximate with a finite polynomial series. The expected solution for the lambertian at this spatial point for the cases

of  $c=.5$  and  $c=.9$  would be similar to figure 4-5, with more backscatter in the  $c=.9$  case than the  $c=.5$ . As a result, the approximating function generated by the legendre polynomials changes less rapidly about  $u=0$  for  $c=.9$  than for  $c=.5$ , and can be constructed with less polynomials.

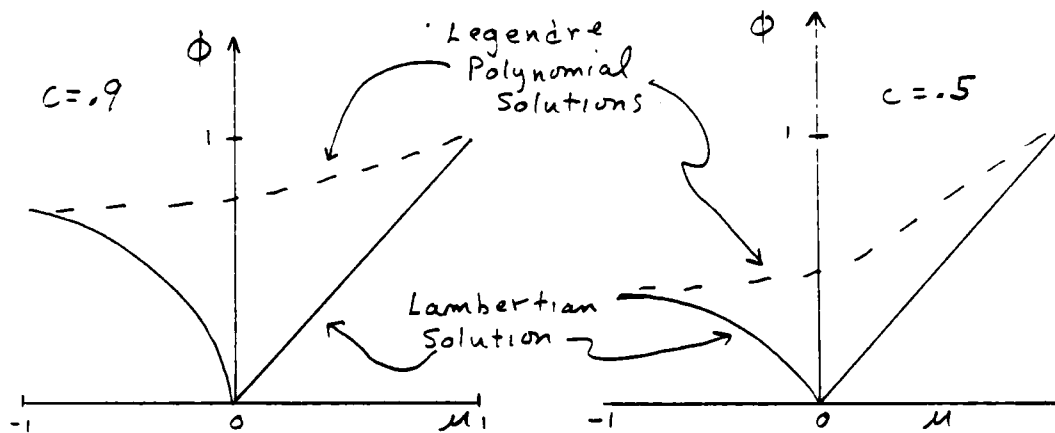


Figure 4-5  
Expected Solution at  $x=0$  for the Lambertian Source  
and Expected Legendre Polynomial Approximations

Used as finite element left hand boundary conditions are the legendre polynomial values of angular flux in appendix H for  $X=0$  and  $u>0$ . With these boundary conditions the finite element solution was tested, and its results compared to the spherical harmonics solution throughout the regions, of varying depth, and with varying cross sections, under scrutiny.

#### D. Results

Penalty functions are guaranteed to be positive with this method since the value of the functional is the integral of a quantity squared.

$$I = \frac{1}{2} \int_D (\mathcal{L}\phi - s)(\mathcal{L}\phi - s) \quad (1-11)$$

If a negative penalty occurs, it is an indicator of error. In the case of no scatter, every penalty was greater than zero because flux was approximated as a cubic, and the integration was exact. In the scattering case, numerical evaluation of the scattering integrals is hardly exact, nor is approximating a hexadic with a cubic, and then analytically performing the integral. Negative penalties could occur, and they would indicate error in evaluating the scattering integral.

The global matrix is guaranteed to be positive definite. In the streaming case it always was positive definite, again due to the exactness of the integration. In the scattering case, a non positive definite global matrix is another indicator of error in scattering integral evaluation. This type of matrix could be solved, and the solution might be fairly accurate, but a desirable characteristic of the finite element method is that the resulting set of linear equations has a positive definite coefficient matrix, since it can be solved quickly and accurately by direct means. Other than positive definite matrices solution techniques must rely upon iterative solution methods, or very long direct schemes, therefore this study insists that the means used to evaluate scattering results in positive definite global coefficient matrices.

#### Numerical Results

Both negative penalties and non positive definite matrices were common with the three numerical techniques used. Simpsons rule was used first. For simple meshes (meshes 1-4) positive definite global matrices occurred. For any further refinement,

error in the integration grew, and the matrix became non positive definite. Since Weddle's rule fits a cubic, it was tried next, and more refinement could occur until the same effect happened. Weddle's rule for  $n=6$  was the last numerical technique tried, and its error causes non positive definite matrices with around 15 triangles per mean free path at  $c=.5$ . In table 4-1 are results for Weddle's  $N=6$  rule in mesh D with a depth of 3 mean free paths and  $c=.5$ . It shows that the method does not provide acceptable accuracy. It seems odd that mesh refinement would increase error. What is occurring is that as the number of triangles is increased, the numerical integration must be performed more often. The error accumulates until it destroys the global matrices positive definiteness. This is even more apparent if  $c=.9$  is used; the scattering integral's contributions are greater, and even less refined meshes produce negative definite matrices. Numerical integration of the scattering integrals holds no potential. Orthogonal relations could be tried, they are used successfully in the  $S_n$  method, but they would probably not be the solution. In the  $S_n$  method, iteration throughout the mesh must occur to reach the proper solution. The finite element technique, as formulated in this study, is not adaptive to iterative, or "marching" methods.

#### Cubic Approximation

Comparison of finite element and PN solution for  $c=.5$  and  $c=.9$  were conducted. Two types of boundary conditions were tried. First, only fluxes were specified and secondly fluxes and its derivatives with respect to  $u$  were specified. Derivatives

ED WCOUT

LI,1,5

1 ==> CO MSHE3.5C MESH

2 ==> XE

3 IER IS ... 0

4 NTRIA N SIGMAS

5 46 151 0.500

LI,276,50

276	COORDINATES		CURRENTS		FIN ELEM	Legendre	
277	X	U	X	U	FLUX	PN FLUX	% DIFF
278	0.000	1.000	-0.849	0.988	1.014	1.014	0.000
279	0.000	0.750	-0.806	0.976	0.767	0.767	0.000
280	0.000	0.500	-0.731	0.983	0.526	0.526	0.000
281	0.000	0.250	-0.441	0.810	0.275	0.275	0.000
282	0.000	0.000	0.064	0.617	0.121	0.121	0.000
283	0.000	-0.250	-0.176	0.352	0.135	0.103	31.817
284	0.000	-0.500	-0.110	0.074	0.106	0.101	5.345
285	0.000	-0.750	-0.088	0.045	0.091	0.074	23.119
286	0.000	-1.000	-0.083	0.219	0.072	0.052	38.357
287	0.750	1.000	-0.457	0.859	0.542	0.533	1.802
288	0.750	0.750	-0.369	0.656	0.349	0.343	1.757
289	0.750	0.250	-0.085	0.191	0.107	0.095	12.497
290	0.750	0.000	-0.033	0.167	0.093	0.064	46.769
291	0.750	-0.250	-0.046	0.104	0.068	0.052	30.086
292	0.750	-0.750	-0.031	0.006	0.048	0.037	26.993
293	0.750	-1.000	-0.043	0.306	0.025	0.033	25.721
294	1.500	1.000	-0.256	0.694	0.290	0.273	6.264
295	1.500	0.500	-0.100	0.252	0.083	0.074	11.697
296	1.500	0.000	0.018	0.091	0.035	0.030	15.972
297	1.500	-0.500	0.001	0.126	0.023	0.020	15.874
298	1.500	-1.000	-0.004	0.373	-0.001	0.016	103.227
299	2.250	1.000	-0.134	0.456	0.150	0.139	7.686
300	2.250	0.750	-0.074	0.192	0.072	0.069	4.287
301	2.250	0.250	-0.015	0.042	0.019	0.019	4.260
302	2.250	0.000	0.011	0.112	0.010	0.014	30.249
303	2.250	-0.250	-0.005	0.049	0.014	0.011	28.081
304	2.250	-0.750	-0.012	0.016	0.013	0.008	58.603
305	2.250	-1.000	0.006	0.214	-0.001	0.007	119.351
306	3.000	1.000	-0.068	0.251	0.075	0.071	6.296
307	3.000	0.500	-0.014	0.044	0.016	0.014	11.580
308	3.000	0.000	-0.013	0.005	0.007	0.007	0.000
309	3.000	-0.250	-0.009	0.004	0.005	0.005	0.000
310	3.000	-0.500	-0.010	0.003	0.004	0.004	0.000
311	3.000	-0.750	-0.010	0.002	0.004	0.004	0.000
312	3.000	-1.000	-0.002	0.002	0.003	0.003	0.000
313	AVERAGE % DIFFERENCE IS .. 19.07682837						
314	FOR AN AVERSGE OF 15.333 TRIANGLES PER MEAN FREE PATH						
EOT..	26.69% For points not specified by boundary cond's						
UP							

Table 4-1

Weddle's Rule n=6 Results for Mesh D, with Range=3.0,  
u Derivatives and Fluxes Specified on the Boundary, c=.5

were found by the use of difference equations on the Pn data. A total of four meshes, A through D were used (appendix F). A, B, and C meshes all have a depth of 3 mean free paths. Mesh D depth was varied from 1 to 5 mean free paths. Since data from these meshes is extensive, selected output is displayed in appendix A, and results are summarized in table 4-2.

The results of table 4-2 indicate that convergence is occurring for  $c=.9$  data only after excessive mesh refinement. The data for  $c=.5$  indicates convergence of the finite element code is occurring, but not to the Pn solution. Specifying u derivatives speeds up convergence. Penalties, expounded as being so important in chapter 3, appear to carry no useful information.

Both boundary conditions are appropriately specified. It is customary in the widely used Pn and Sn transport codes, to specify only fluxes. In general these codes do not directly use the u derivatives on boundary. However if the flux is known as a function of u at a specific spatial location, then certainly the flux derivative with respect to u is known at that point. Since the finite element code uses  $\phi_u$  as an interpolation node, specifying its value on the boundary is appropriate, and can only speed convergence to the same solution.

The lack of exactness in scattering integral evaluation has destroyed element, and total penalty usefulness. Consider the origin of a particular element's penalty, pen(i)

$$\text{pen}(i) = \hat{\phi}_i \underline{M}_L \phi_i + \hat{\phi}_i \sum_{\substack{j=\text{top} \\ \text{column } \Delta}}^{\text{bottom } \Delta} \underline{NLM}(ij) \phi_j \quad (4-21)$$

= streaming and absorbing + scattering  
contribution contribution

The streaming and absorbing component is always positive. It

c=.5

Mesh	Depth(mean free paths)	# triangles per mfp	Avg perc diff	Total penalty	Sum of Abs(pen)
D	1	46	7.81	.51E-5	.78E-2
D	2	23	7.37	-.53E-5	.87E-2
D	3	15.3	7.85(8.91)	-.36E-4	.87E-2
D	4	11.5	9.34	-.11E-3	.85E-2
D	5	9.2	13.5	-.25E-3	.82E-2
C	3	13.3	26.2 (7.38)	-.94E-4	.47E-2
B	3	4.0	* (22.53)		
A	3	1.3	21.4(64.51)	-.32E-2	.92E-2

C=.9

Mesh	Depth(mean free paths)	# triangles per mfp	Avg perc diff	Total penalty	Sum of Abs(pen)
D	1	46	1.11	.10E-5	.82E-2
D	2	23	1.27	-.11E-4	.11E-1
D	3	15.3	3.88(1.59)	-.47E-4	.11E-1
D	4	11.5	14.89	-.13E-3	.10E-1
D	5	9.2	45.79	-.31E-3	.86E-2
C	3	13.3	75.46(1.28)	.40E-4	.15E-2
B	3	4.0	* (6.69)		
A	3	1.3	58.0(18.91)	-.23E-2	.10E-1

Table 4-2

Cubic Approximation of Scattering Integral Results  
Compared with Legendre Polynomial Solution for c=.5 and  
c=.9. Average Percent Difference of Nodal Values Other than  
Those Specified as Boundary Conditions, with flux only as a  
Boundary Condition. Values in Parenthesis are Same Meshes  
with Flux and u Derivative Specified. \* is Non Positive  
Definite Global Matrix.

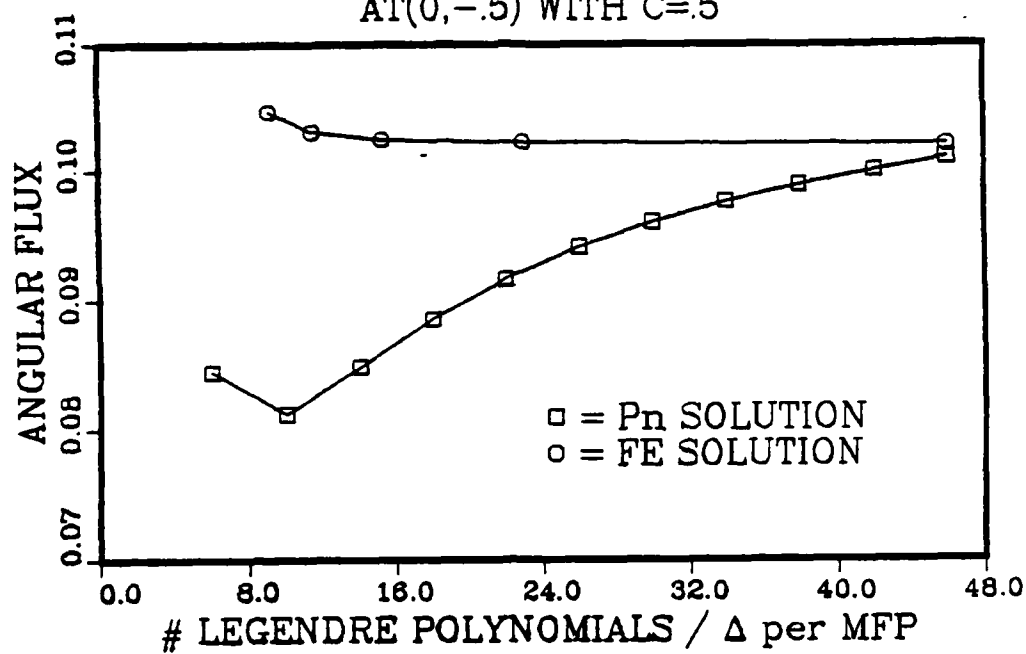
exactly this that constitutes penalties in the case of no  
scatter. The scattering component is expected to be negative,  
as can be seen by evaluating the signs of the integral  
coefficient constants of equation (4-3),  $(\frac{\xi_s^2}{2} - \xi_s \xi_t)$  and  $(-\xi_s)$   
are both less than zero. The sum of the streaming and  
scattering penalty contributions should remain positive however,

since they represent the square of a quantity. When scattering evaluation is with error, its penalty contribution can grow too large, and an element's penalty drops below zero. If this happens, summing of element penalties for a total mesh penalty leads to misleading information. It was thought that the magnitude of a penalty might carry the desired information on a fit's correctness, so the sum of penalty absolute values was computed. Comparison of this data, displayed in table 4-2 also lacks the desired information. Negative element penalties are in every instance associated with triangles where a large amount of scattering, and a small amount of streaming is occurring. Because the scattering integral evaluation is inexact, the penalty function has lost its value.

Graphs of figures 4-6 and 4-7 compare finite element solutions with the legendre polynomial solution, for various triangle densities and numbers of legendre polynomials being used. All finite element computations on the graphs were done with mesh D, varying the depth to change triangle densities. It appears from this data that with more legendre polynomials the finite element and  $P_n$  solutions would be exact. Convergence is faster in the  $c=.9$  case because the larger backscatter creates a smoother flowing function, able to be approximated with fewer legendre polynomials than the more rapidly changing  $c=.5$  solution. Boundary conditions, used in the finite element code as specified by the spherical harmonic solution, have not settled down yet either, as shown in table 4-3.

Based upon this information it appears that the finite

FIGURE 4-6  
COMPARISON OF FE AND Pn SOLUTION  
AT(0,-.5) WITH C=.5



AT(0,-.25) WITH C=.5

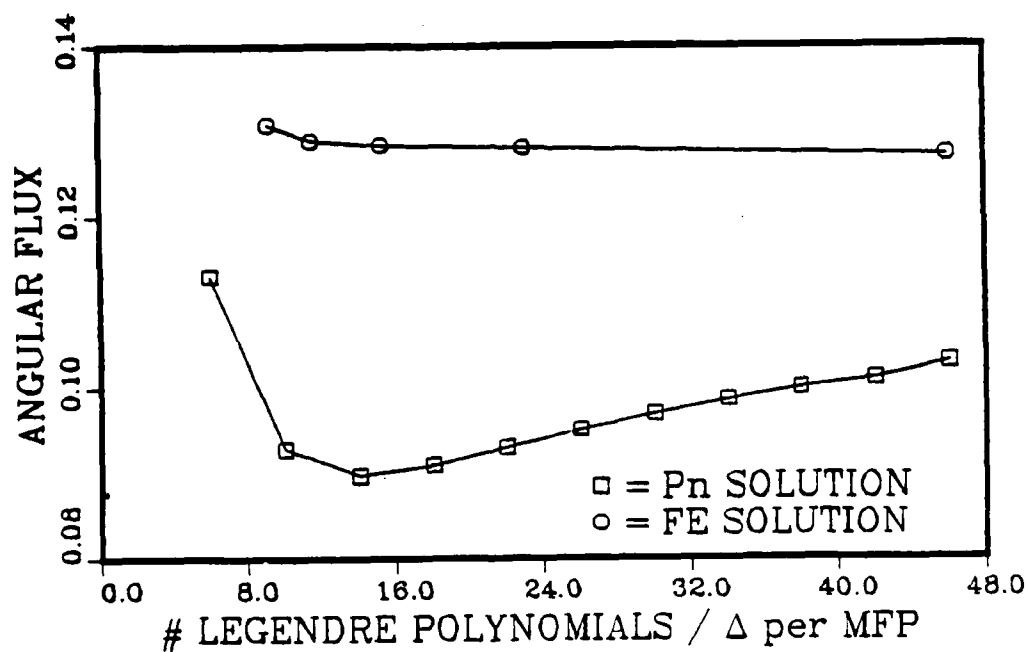


FIGURE 4-7  
COMPARISON OF FE AND Pn SOLUTION  
AT(0,-.25) WITH C=.9

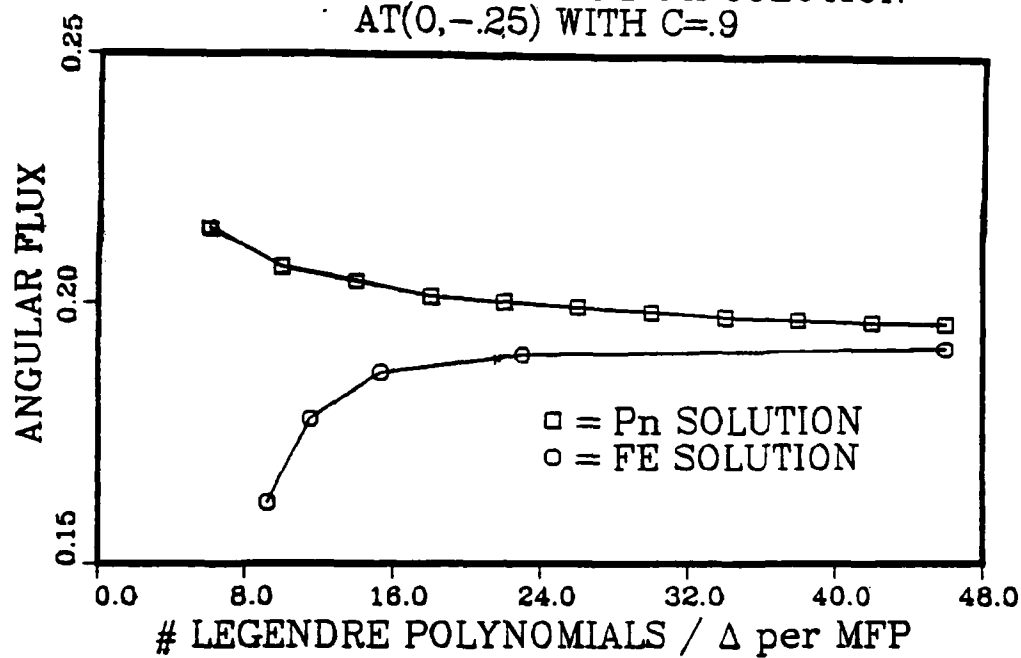
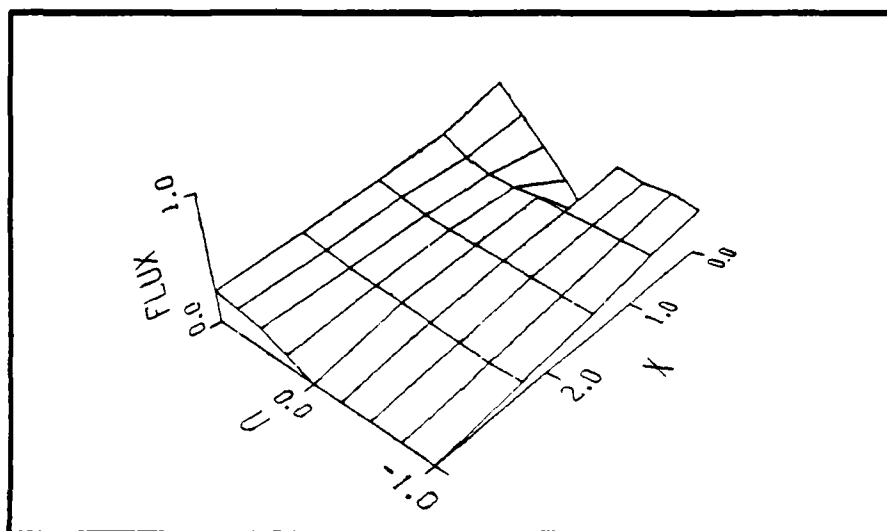


FIGURE 4-8  
ANGULAR FLUX FROM A LAMBERTIAN  
SCATTERING ONLY MEDIUM



(x,u)	c	change of flux	% change
(0,.5)	.5	4.6E-3	.87
0,.5	.9	1.1E-3	.33
0,.25	.5	7.6E-3	2.7
0,.25	.9	2.1E-3	.68
3,-1	.5	6.5E-5	1.9
3,-1	.9	1.0E-6	3.5E-3

Table 4-3  
Pn Predicted Flux Rate of Change of Selected  
Boundary Points Over Polynomials 30-46

element calculations are successfully predicting angular flux. Under these circumstances it is difficult to determine the amount of refinement required for convergence, but it appears that if fluxes only are specified on boundaries the method converges with 15 to 20 triangles per mean free path. If fluxes and derivatives are specified, convergence occurs with 10 - 15 elements per mean free path. Less angle refinement is also required if derivatives are specified on boundaries. This is approximately the same degree of refinement as an S4 calculation with two spatial nodes per mean free path. Positive definite matrices are not guaranteed ( as in the case of mesh B.).

The only difference between mesh C and D is refinement over angle in the first and last columns. Close analysis of table 4-2 data shows that this angle refinement is more important than spatial refinement when fluxes only are used as boundary conditions. This is further indication of scattering term inexactness. The scattering calculations error can be estimated from  $c=.9$  data of table 4-2. With 46 triangles per mean free path, the average nodal percent difference of 1.11% can be

Pen - element penalty

G1, G2, G3 - derivatives of triangular coordinates w.r.t. space

F1, F2, F3 - derivatives of triangular coordinates w.r.t. angle

X1,X2,X3,U1,U2,U3 - specific coordinates of the triangle under  
scrutinies geometric nodes

V - Array storing the integral of the twenty tetrahedral  
coordinate combinations which together form a complete  
basis for a cubic in three dimensions (2-41). Row two has  
the integral of times (2-41), row three times (2-  
41) , rows 4 and 5 contain and times (2-41)  
integrated over tetrahedral volume respectively.

SGM - M5, M6, M7, and M8 of (2-42) and M18 of (2-43)

E, F, G, - arrays of dimension 4 storing the derivatives of the  
four tetrahedral coordinates w.r.t. space, incident angle and  
scattered angle respectively

H - the basis functions for each of the 5 scattering integrals  
(expansion of u requires that the second integral be done  
four separate times)

SA - the first scattering integral matrix

SB - the second scattering integral matrix

#### Integers Passed as Arguments

N - number of nodes

TRI - local triangle

TRIP - non local triangle

NTRIA - number of triangles

## Appendix A - Program Listing

### Glossary of Variables

#### Variables Passed as Common

MG - Global matrix

ML - local matrix

NLM - non local matrix

GT - matrix of interpolating function constants

#### Variables Passed as Double Precision Arguments

Cordnd - cartesian (x,u) coordinates of finite element nodes

Phi - angular flux

Areas - triangle areas

MA - absorbing matrix

SC1, SC2 , ... SC6 - coefficients of streaming matrices per  
appendix D

SR1, SR2, ... SR6 - per appendix D, row matrices to augment SC  
matrices

BC1, BC2, BC3, BR1, BR2 , BR3 - coefficients of boundary  
matrices per appendix C

MB - boundary matrix

MS - streaming matrix

DRVS - matrix of derivatives, overlayed on boundary term  
coefficients per appendix C

Range - depth, in mean free paths, of region under scrutiny

SIGMAT -  $\sum_t$

SIGMAS -  $\sum_s$

### Bibliography

1. Duderstadt, James J. and William R. Martin, Transport Theory, New York, John Wiley & Sons, 1979
2. Goff, Alan D., A Finite Element Solution of a Self Adjoint Transport Equation in One Dimension, Masters Thesis, Air Force Institute of Technology, 1984. (AFIT/GNE/PH/84M-4)
3. Huebner, Kenneth H., and Earl A. Thornton, The Finite Element Method For Engineers, John Wiley & Sons 1982.
4. Kreysig, Erwin, Advanced Engineering Mathematics, John Wiley & Son, 1983.
5. Lewins, Jeffery. Importance, The Adjoint Function, Pergamon Press Ltd. Norwich, England 1965.
6. Strang, Gilbert, and George Fix, An Analysis of the Finite Element Method, Englewood Cliffs, N.J., 1973.
7. Westlake, Joan R., A Handbook of Numerical Matrix Inversion And Solution of Linear Equations, John Wiley & Sons, New York, 1968

Any interpolant that uses field variable derivatives as finite element interpolation nodes has basis functions that are geometry dependent, and increases calculations significantly. This type of interpolant was accepted for the local terms because the increase in accuracy made up for the extra calculations. It is not necessary to use a geometry dependent interpolating function for the nonlocal terms, and this type of approximation holds no accuracy benefits. Exact scattering term evaluation is possible with geometry independent interpolants, and is recommended as any subsequent study's first effort.

interpolants.

The streaming results clearly show the penalty function's usefulness. Not only is the global penalty a faultless indicator of accuracy, element penalties may be used to dictate where local refinement should occur.

Two methods were used to evaluate the scattering terms, and analysis of their results leads to a proposal for a third integration technique, which should be both more efficient and accurate. Numerical techniques, of accuracy up to Weddle's for  $n=6$  were unsuccessful. Cubic approximation of the hexadic scattering integral was accurate, required slightly more refinement than expected, and appears to be computationally excessive. Worst of all, the inexactness of the scattering integral evaluation destroys penalty value, and does not guarantee positive definite global matrices. Chapter 5 describes proposed exact hexadic integration, with geometry independent basis functions that should significantly reduce computations, return penalty usefulness, and insure positive definiteness. With exact scattering integral evaluation, accuracy equal to the streaming case should be achieved with comparable mesh refinement.

Extensions to other than isotropic scatter will be straightforward. If the scattering kernel is expanded in terms of a legendre polynomial series as it ordinarily is, the scattering integrals would be slightly more complicated, but achievable. Integration with  $dx$ ,  $du$  and  $du'$  over a four node tetrahedron would still result, only the form of the function being integrated would be changed.

## 6. Conclusion

The finite element method has been very successful in a variety of fields. It was felt that since the self adjoint reformulation of the transport operator could be expressed as a quadratic functional, finite elements could be applied successfully to transport problems. Concisely stated, the result of this study is that the method works, and that it appears to hold potential for very accurate solutions with moderately refined meshes. The present digitization of the method, described in this document, and written in appendix A, bears improvement, both in accuracy and computational efficiency.

It was found that with linear interpolants the method converged in the case of no scatter, with around 25 triangles per mean free path for  $u > 0$ . Linear interpolants were not tested in the scattering case, but straightforward extension of the streaming results suggests that at least 50 triangles per mean free path will be required to reach an accurate solution. This is an enormous amount of refinement. The  $C^0$  quadratic fit was only slightly better. Unfortunately columnar mesh restriction destroyed a semi  $C^1$  fit, and cubic interpolants were used. These are very powerful in the streaming case, achieving accuracy of greater than 99% with around 4 triangles per mean free path. Codes used in this study were not written with the intention of comparing speeds. Run time comparisons are therefore not absolute, but they do indicate that the more accurate fit is not computationally excessive, and may even require less cpu time to converge than either of the  $C^0$

and

$$\phi_x = \tilde{h}_x \phi$$

(5-2)

where  $\underline{h}$  and  $\underline{h}_x$  in this instance represent the dimension (10) distinct basis functions and their spatial derivatives of the cubic fits over a triangle, found while calculating the local terms.

Polynomial	Quantity	Polynomial	Quantity
$L_i^6$	4	$L_i^3 L_j^2 L_k$	24
$L_i^5 L_j$	12	$L_i^3 L_j L_k L_l$	4
$L_i^4 L_j^2$	12	$L_i^2 L_j^2 L_k^2$	4
$L_i^4 L_j L_k$	12	$L_i^2 L_j^2 L_k L_l$	6
$L_i^3 L_j^3$	6		

Table 5-1

84 Polynomials for Three Dimensional Hexadic

### C. Summary

Results of chapter 4 dictate the need for exact scattering integral evaluation. The hexadic using flux only as degrees of freedom will integrate exactly, and probably reduce computations. Time precluded digitization of this fit, and it is recommended as the first effort of any subsequent study.

tetrahedron of figure 5-1 into six layers of equal height. Natural coordinates of these nodes can be computed using 2-38 and the matrix  $\underline{GT}$  can be found by the method described in chapter 2.

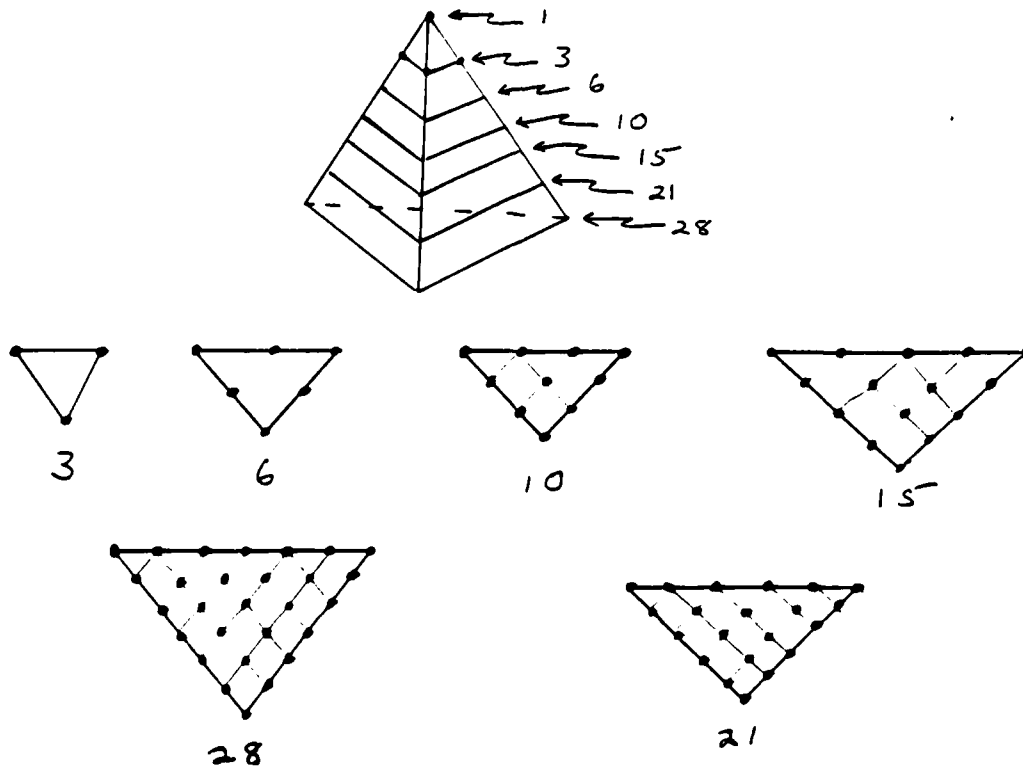


Figure 5-1  
84 Flux Interpolation Nodes of Hexadic Three  
Dimensional Fit

The 84 polynomials, which together constitute a complete basis for the hexadic are given in table 5-1, with quantities indicated.

With this information the basis functions are specified. The degrees of freedom  $F = \phi\phi'$  and  $G = \phi_x\phi'$  are distinct for each tetrahedron.  $\phi$  and  $\phi_x$  need to be calculated only once for each triangle with

$$\phi = \tilde{h} \underline{\underline{\psi}} \quad (5-1)$$

## 5. Exact Scattering Integral Evaluation

Chapter 4 results show that the finite element method, in the case of isotropic scatter works, but one would like to see it converge with less mesh refinement, and with a smaller number of computations. A method of exactly integrating the scattering terms is explained in this chapter that should meet this objective, as well as restore the penalty function's usefulness and guarantee positive definite matrices.

### A. Hexadic Interpolation With Flux

A hexadic function in three dimensions requires 84 degrees of freedom to be completely specified. If all are flux, then they can be described in terms of the twenty nodal two dimensional cubic interpolants (ten from each triangle), independent of tetrahedral geometry. That is to say, the basis functions would be constant, since they no longer involve derivatives of natural coordinates. There are five distinct integrals to be performed, because of the  $u$  expansion in the second scattering integral. Basis functions can be calculated separately, and stored in a single matrix of dimension (5,84). This significantly reduces calculations, and eliminates the requirement for the finite element transport code to find three dimensional interpolants entirely.

### B. Interpolation Nodes and Basis Functions

The following nodes are evenly volume distributed and should provide a good hexadic fit. Consider slicing the

derivatives of the flux on boundaries.

The penalty function's usefulness has been ruined by inexact scattering integral evaluation.

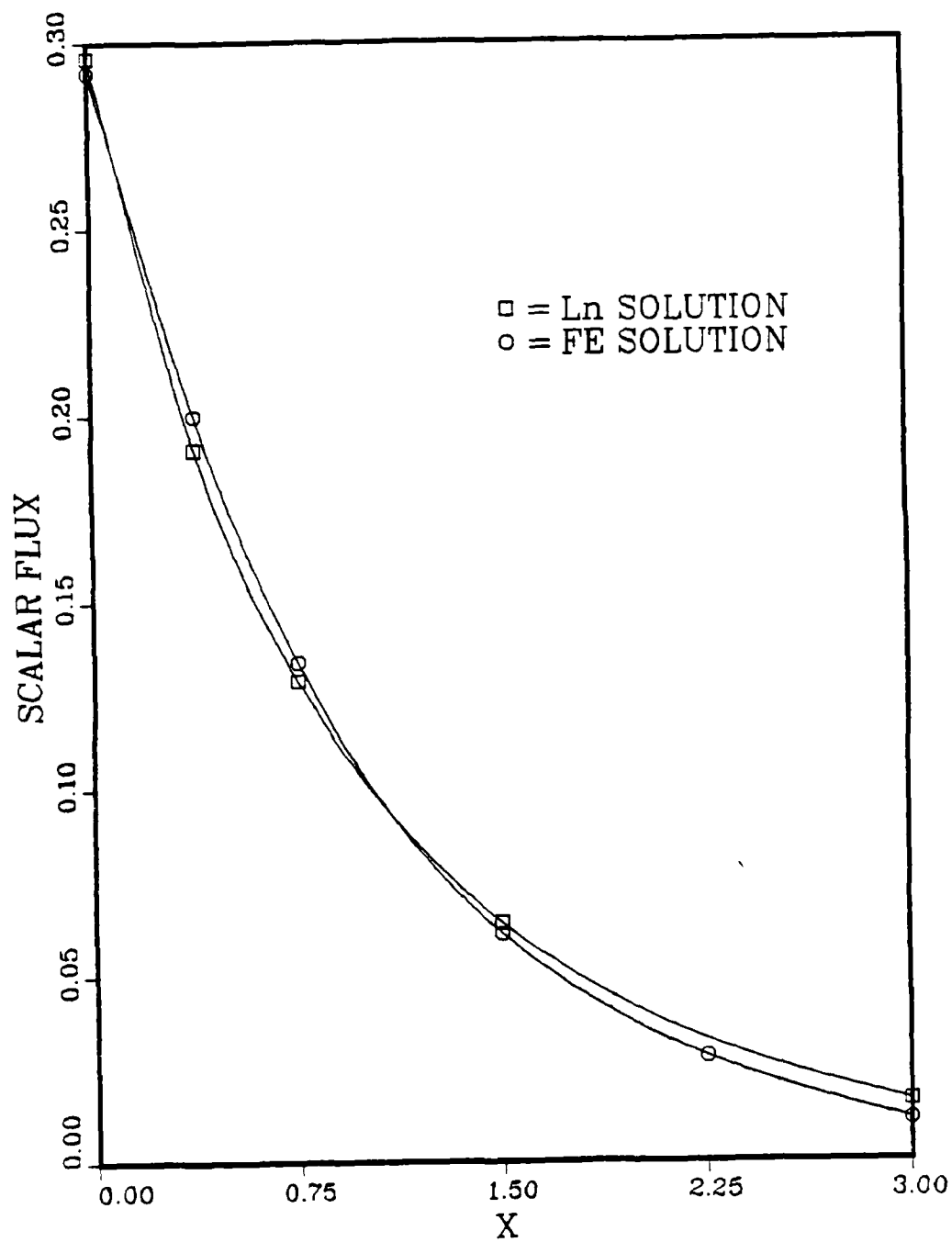
element mesh D results in nearly 800 tetrahedra over which the scattering integrals must be evaluated. Each of these tetrahedra, treated in the code as geometrically distinct, require separate interpolation functions, and this is the probable cause of calculational excesses.

#### Summary

When scattering occurs, the variational integral is evaluated by integrating over space, angle, and scattered angle. To simplify this calculation triangles are constrained in this study to columns. Since cubic interpolating functions are used for flux, the scattering integrals involve the product of two cubics, or hexadics. Mapped in three dimensions, the local and nonlocal triangles create tetrahedra.

Two methods were tried to evaluate these integrals. Strict numerical evaluation with relations of accuracy up to Weddle's for  $n=6$  did not obtain acceptable accuracy. Error with these techniques was cumulative, and refinement resulted in a loss of the global matrices positive definiteness with around 15 triangles per mean free path, prior to convergence. Numerical evaluation of the scattering integrals appears to hold no potential with the method's present formulation. Approximating the hexadic with another cubic gave better results, but did not guarantee positive definiteness. Solution accuracy was sufficiently verified against a Pn benchmark over the test domain. Convergence appears to occur with a reasonable but larger amount of mesh refinement than in the no scattering case. The number of computations needing to be performed may be excessive. Convergence is speeded by specifying angle

FIGURE 4-9  
COMPARISON OF  $L_n$  AND FE SCALAR FLUX  
LAMBERTIAN SOURCE, WITH  $C=5$



finite element angular flux was integrated over angle with the assistance of IMSL routine ICSCCU, cubic spline interpolation and

$$\text{Scalar Flux} = \frac{1}{2} \int_{-1}^1 du \phi(x, u) \quad (4-22)$$

A comparison of the Ln and FE results for mesh D, with a depth of three mean free paths, is displayed in table 4-4, and graphed in figure 4-9.

x	0	.375	.75	1.5	2.25	3.0
Ln	.296	.191	.129	.064	c	.016
FE	.292	.200	.134	.061	.028	.011

Table 4-4  
Ln and Finite Element Comparison of Scalar Fluxes  
Lambertian Source, c=.5, Mesh D, Fluxes and Derivatives  
Specified as Boundary Conditions

Agreement between the two codes is good. Differences are of the same order magnitude as the scattering error estimation previously done for this mesh. At x=3, the percentage difference is large, but the magnitude of the variation is small. The graph of figure 4-9 displays the close correlation between the two separate calculational results.

Computationally the method can be considered excessive. Mesh E, composed of 46 elements, requires over 4 minutes of CPU time on a Harris 800 computer. The correlation between Harris times and the Vax times of chapter 3 is unknown, but clearly the number of calculations has greatly increased. The 4 column 46

considered as entirely due to truncation of the polynomial series. Mesh D calculations, with a depth of three mean free paths, and no scattering show an average of 0.12% difference at  $u=1$  from analytically computed angular flux. This represents the error from cubic approximation of flux, for the mesh, and degree of refinement under scrutiny. Comparing this to the scattering mesh D case of three mean free paths leaves a remainder of 2.65%, an approximate estimate of scattering integral evaluation error in this case.

Table 4-2 contains 3 instances where less refined meshes appear to give more accurate answers than a denser mesh. If penalties were exact they should indicate, as in the no scattering case, that better finite element fits can occur without necessarily observing steady convergence of nodal values to an "exact" answer.

Further indication of the finite element methods success comes from investigating the lambertian flux incident on the left boundary with  $c=1.0$ . The angular flux in this scattering only medium of depth equal to three mean free paths reflects the hump predicted at  $x=0$  of figure 4-5. The surface of angular flux, plotted in figure 4-8 shows that particles leak out both ends, and that angular flux is approaching isotropy as the region is penetrated.

Cited in Goff's thesis (2:67), were the benchmark case results of a transport code known as Ln. This a program recently developed as a P.H.D. dissertation by LCDR. Kirk A. Mathews (AFIT/GNE/85D). The output of this code is scalar flux, so the

CASE - integer reflecting the orientation of local and non local triangles w.r.t. each other

TIME - integer reflecting which half of case 2 and case 4 is being currently calculated

PTNODE - array storing the global numbering of a triangles finite element interpolation nodes

COLUMN - array storing the column each triangle belongs to, the top element of that column, and the number of elements the column possesses

Variables, Not Passed, by Subroutine, Requiring Definition

Subroutine SINFCN

SGT - matrix of interpolating function constants for the tetrahedral cubic (2-43)

M - array storing the 4x4 partitioned matrices of (2-42) and (2-43)

Subroutine SCATA and SCATB

W1,W2,W3,W4,W5,W6 - dimension 10 vectors storing local and non local flux, and its derivatives, at locations that are not triangular cubic interpolation nodes

F - array storing the twenty 10x10 matrices used as interpolation nodes for the three dimensional cubic

```

LI,1,2500
1  PROGRAM FECUBE
2  * FINITE ELEMENT SOLUTION OF ONE SPEED TRANSPORT EQUATION IN
3  * SLAB GEOMETRY, ISOTROPIC SCATTER, CUBIC APPROXIMATION OF
4  * FLUX, CUBIC APPROXIMATION OF HEXADIC SCATTERING INTEGRAL
5
6  PARAMETER (MNODE=151 , MNTRIA=50)
7
8  DOUBLE PRECISION CORDND(MNODE,2),PHI(MNODE)
9  DOUBLE PRECISION AREAS(MNTRIA),MA(10,10)
10 DOUBLE PRECISION SC1(10,33),SR1(18),SC2(10,33),SR2(18)
11 DOUBLE PRECISION SC3(10,33),SR3(18),SC4(10,33),SR4(18)
12 DOUBLE PRECISION SC5(10,33),SR5(18),SC6(10,33),SR6(18)
13 DOUBLE PRECISION BC1(10,20),BR1(10)
14 DOUBLE PRECISION BC2(10,20),BR2(10),D1,D2
15 DOUBLE PRECISION BC3(10,20),BR3(10),AS(MNODE*(MNODE-1)/2)
16 DOUBLE PRECISION ML(MNTRIA,10,10)
17 DOUBLE PRECISION NLM(MNTRIA,16,10,10),NLI(MNTRIA,4,10)
18 DOUBLE PRECISION MG(MNODE,MNODE)
19 DOUBLE PRECISION GT(MNTRIA,10,10),LI(MNTRIA,10,4)
20 DOUBLE PRECISION MB(10,10),MS(10,10),DRVS(10,2)
21 DOUBLE PRECISION RANGE,SIGMAT,SIGMAS,PEN(MNTRIA)
22 DOUBLE PRECISION G1,G2,G3,F1,F2,F3,A
23 DOUBLE PRECISION U1,U2,U3,X1,X2,X3
24 DOUBLE PRECISION V(5,20),SGM(5,4,4)
25 DOUBLE PRECISION E(4),F(4),G(4),H(5,20),SA(10,10),SB(10,10)
26 INTEGER N,TRI,TRIP,NTRIA,CASE,TIME
27 INTEGER PTNODE(MNTRIA,11),COLUMN(32,2)
28 LOGICAL CHECK1
29 COMMON MG,ML,NLM,NLI,LI,GT
30
31 CHECK1 = .FALSE.
32
33 * READ INITIAL DATA
34 CALL GDATA(NTRIA,N,PTNODE,COLUMN,CORDND,
35 C AREAS,RANGE,SIGMAT,SIGMAS,MA,BC1,BR1,BC2,BR2,BC3,BR3,
36 C SC1,SR1,SC2,SR2,SC3,SR3,SC4,SR4,SC5,SR5,SC6,SR6,
37 C V,SGM,PHI)
38
39
40 * RENUMBER THE MESH, GLOBALLY, AND LOCALLY PER FIGURE 2-4
41 CALL CHGRID (PTNODE,CORDND,N,NTRIA)
42
43
44 * ZERO THE GLOBAL MATRIX
45 DO 69 I=1,N
46 DO 68 J=1,N
47 MG(I,J)=0.0
48 68 CONTINUE
49 69 CONTINUE
50
51 * CALCULATE PARTICLE STREAMING,ABSORBING AND BOUNDARY TERMS
52 * ASSEMBLE INTO LOCAL MATRIX FOR A TRIANGLE, AND ASSEMBLE
53 * GLOBALLY
54 DO 50 TRI=1,NTRIA
55 U1=CORDND(PTNODE(TRI,1),2)

```

```

56      U2=CORDND(PTNODE(TRI,4),2)
57      U3=CORDND(PTNODE(TRI,7),2)
58      X1=CORDND(PTNODE(TRI,1),1)
59      X2=CORDND(PTNODE(TRI,4),1)
60      X3=CORDND(PTNODE(TRI,7),1)
61      A=AREAS(TRI)*2.0
62      G1=(U2-U3)/A
63      G2=(U3-U1)/A
64      G3=(U1-U2)/A
65      F1=(X3-X2)/A
66      F2=(X1-X3)/A
67      F3=(X2-X1)/A
68      CALL INFCN(TRI,G1,G2,G3,F1,F2,F3)
69      CALL BNDRY (U1,U2,U3,G1,G2,G3,BC1,BC2,BC3,BR1
70      C      ,BR2,BR3,SIGMAT,MB,DRVS,AREAS,TRI)
71      CALL STREAM(SC1,SR1,SC2,SR2,SC3,SR3,SC4,SR4,SC5,SR5,
72      C      SC6,SR6,MS,U1,U2,U3,G1,G2,G3,AREAS,TRI,
73      C      DRVS)
74      CALL LMATRX(MA,MB,MS,AREAS,SIGMAT,TRI)
75      CALL ASEMBL(PTNODE,TRI)
76 50    CONTINUE
77
78 * CALCULATE SCATTERING CONTRIBUTION - FOR A TRIANGLE - FROM
79 * COLUMN TOP TO BOTTOM
80      DO 150 TRI=1,NTRIA
81          K=COLUMN(PTNODE(TRI,11),1)
82          DO 125 TRIP=K,K-1+COLUMN(PTNODE(TRI,11),2)
83              TIME=1
84 130      CALL CASEDT(TRI,TRIP,CORDND,PTNODE,TIME,E,F,G,
85      C      V6,CASE,U1,U2,U3,X1,X2,X3)
86              CALL SINFCN(E,F,G,V,SGM,H)
87              CALL SCATA(H,TRI,TRIP,CASE,TIME,SA,CORDND,PTNODE)
88              CALL SCATB(U1,U2,U3,X1,X2,X3,TRI,TRIP,AREAS,H,
89      C      CASE,TIME,SB,CORDND,PTNODE)
90              CALL NLMTX(TRI,TRIP,SIGMAS,SIGMAT,
91      C      TIME,V6,SA,SB)
92              IF (CASE.EQ.2.OR.CASE.EQ.4) THEN
93                  IF (TIME.EQ.1) THEN
94                      TIME=TIME+1
95                      GO TO 130
96                  ENDIF
97              ENDIF
98              CALL SASMBL(PTNODE,TRI,TRIP)
99 125      CONTINUE
100 150      CONTINUE
101
102 * PUT GLOBAL MATRIX IN ITS QUADRATIC FORM
103      DO 250 I=1,N
104          DO 200 J=1,I
105              MG(I,J)=(MG(I,J)+MG(J,I))/2.0
106              MG(J,I)=MG(I,J)
107 200      CONTINUE
108 250      CONTINUE
109
110 * IF DESIRED, DIAGNOSTIC DATA CAN BE TURNED ON IN "OUTPUT" HERE
111      CALL OUTPUT(PHI,N,PTNODE,CORDND,NTRIA,CHECK1

```

```

112      C      ,PEN,SIGMAS,RANGE,SIGMAT)
113      CHECK1 = .TRUE.
114
115 * APPLY THE BOUNDARY CONDITIONS
116      CALL BNDEND(CORDND,PHI,N,NTRIA,RANGE)
117
118 * PLACE GLOBAL MATRIX IN BAND STORAGE FOR IMSL
119      K=1
120      DO 350 I=1,N
121          DO 300 J=1,I
122              AS(K)=MG(I,J)
123              K=K+1
124      300      CONTINUE
125      350      CONTINUE
126
127 * SOLVE THE SET OF LINEAR EQUATIONS
128      CALL LEQT1P(AS,1,N,PHI,MNODE,IDGT,D1,D2,IER)
129      PRINT*, 'IER IS ...',IER
130
131 * CALCULATE PENALTIES, AND PRINT OUT RESULTS
132      CALL PENLTY(PHI,PTNODE,PEN,NTRIA,COLUMN)
133      CALL OUTPUT(PHI,N,PTNODE,CORDND,NTRIA,CHECK1
134      C      ,PEN,SIGMAS,RANGE,SIGMAT)
135
136      END
137
138
139 *****
140
141 * GATHER INITIAL DATA - READS THREE DATA FILES
142 * MESH - GRID DATA (APPENDIX F)
143 * CODATA - COEFFICIENTS OF LOCAL MATRICES (APPENDICES B,C,D)
144 * SDATA - CONSTANTS. FIVE OF THE PARTITIONED MATRICES OF 2-42
145 *      AND 2-43, AS WELL AS THE INTEGRALS OF BASIS POLYNOMIALS
146
147      SUBROUTINE GDATA(NTRIA,N,PTNODE,COLUMN,CORDND,
148      C      AREAS,RANGE,SIGMAT,SIGMAS,MA,BC1,BR1,BC2,BR2,BC3,BR3,
149      C      SC1,SR1,SC2,SR2,SC3,SR3,SC4,SR4,SC5,SR5,SC6,SR6,
150      C      V,SGM,PHI)
151
152      PARAMETER (MNODE=151 , MNTRIA=50)
153
154      DOUBLE PRECISION CORDND(MNODE,2)
155      DOUBLE PRECISION AREAS(MNTRIA),MA(10,10)
156      DOUBLE PRECISION SC1(10,33),SR1(18),SC2(10,33),SR2(18)
157      DOUBLE PRECISION SC3(10,33),SR3(18),SC4(10,33),SR4(18)
158      DOUBLE PRECISION SC5(10,33),SR5(18),SC6(10,33),SR6(18)
159      DOUBLE PRECISION BC1(10,20),BR1(10)
160      DOUBLE PRECISION BC2(10,20),BR2(10)
161      DOUBLE PRECISION BC3(10,20),BR3(10)
162      DOUBLE PRECISION V(5,20),SGM(5,4,4)
163      DOUBLE PRECISION RANGE,SIGMAT,SIGMAS,PHI(MNODE)
164      DOUBLE PRECISION ML(MNTRIA,10,10)
165      DOUBLE PRECISION NL(MNTRIA,16,10,10),NLI(MNTRIA,4,10)
166      DOUBLE PRECISION MG(MNODE,MNODE)
167      DOUBLE PRECISION GT(MNTRIA,10,10),LI(MNTRIA,10,4)

```

```

168 INTEGER N,NTRIA,TRI,NB
169 INTEGER PTNODE(MNTRIA,11),COLUMN(32,2)
170 CHARACTER TRASH*21
171 COMMON MG,ML,NLM,NLI,LI,GT
172
173 OPEN(15,FILE='MESH',STATUS='OLD')
174 REWIND 15
175
176 READ(15,'(A16)') TRASH
177 READ(15,'(3(1X,I7))') NTRIA,N,NCOL
178 READ(15,'(1X)')
179
180
181 READ(15,'(A16)') TRASH
182 READ(15,'(3(1X,F7.3))') RANGE,SIGMAT,SIGMAS
183 RANGE=RANGE*SIGMAT
184 READ(15,'(1X)')
185
186
187 READ(15,'(A16)') TRASH
188 DO 60 I=1,NTRIA
189     READ(15,'(1X,I7,8X,4(1X,I7))') TRI,(PTNODE(I,J),J=1,4)
190 60 CONTINUE
191 READ(15,'(1X)')
192
193 READ(15,'(A16)') TRASH
194 DO 70 I=1,NCOL
195     READ(15,'(3(1X,I7,8X))') TRI,(COLUMN(I,J),J=1,2)
196 70 CONTINUE
197 READ(15,'(1X)')
198
199 READ(15,'(A16)') TRASH
200 DO 80 I=1,N
201     READ(15,'(1X,I7,8X,2(2X,F7.3))') NODE,(CORDND(I,J),J=1,2)
202     CORDND(I,1)=CORDND(I,1)*RANGE
203 80 CONTINUE
204 READ(15,'(1X)')
205
206     DO 82 I=1,3*N+NTRIA
207         PHI(I)=0.0
208 82 CONTINUE
209 READ(15,'(A16)') TRASH
210 READ(15,'(I7)') NB
211 DO 83 I=1,NB
212     READ(15,'(1X,I7,8X,E11.5)') J,PHI(J)
213 83 CONTINUE
214
215 CLOSE (15)
216
217 DO 90 TRI=1,NTRIA
218     U3=CORDND(PTNODE(TRI,3),2)
219     U2=CORDND(PTNODE(TRI,2),2)
220     X2=CORDND(PTNODE(TRI,2),1)
221     X1=CORDND(PTNODE(TRI,1),1)
222     AREAS(TRI)=ABS(.5*(U3-U2)*(X2-X1))
223     IF (AREAS(TRI).LT.1.0E-15) THEN

```

```

224      PRINT*, 'AREA OF ZERO IN ELEMENT', TRI
225      ENDIF
226 90    CONTINUE
227
228      OPEN(16, FILE='CODATA', STATUS='OLD')
229      REWIND 16
230      DO 100 I=1,10
231          READ (16, '(10(1X,F5.1))') (MA(I,J), J=1,10)
232 100    CONTINUE
233
234
235
236      DO 110 I=1,10
237          READ (16, '(10(1X,F5.1))') (BC1(I,J), J=1,10)
238          READ (16, '(10(1X,F5.1))') (BC1(I,J), J=11,20)
239 110    CONTINUE
240          READ (16, '(10(1X,F5.1))') (BR1(I), I=1,10)
241
242      DO 120 I=1,10
243          READ (16, '(10(1X,F5.1))') (BC2(I,J), J=1,10)
244
245          READ (16, '(10(1X,F5.1))') (BC2(I,J), J=11,20)
246 120    CONTINUE
247          READ (16, '(10(1X,F5.1))') (BR2(I), I=1,10)
248
249      DO 130 I=1,10
250          READ(16, '(10(1X,F5.1))') (BC3(I,J), J=1,10)
251          READ(16, '(10(1X,F5.1))') (BC3(I,J), J=11,20)
252 130    CONTINUE
253          READ(16, '(10(1X,F5.1))') (BR3(I), I=1,10)
254
255      DO 140 I=1,10
256          READ (16,4200) (SC1(I,J), J=1,10)
257          READ (16,4200) (SC1(I,J), J=11,20)
258          READ (16,4200) (SC1(I,J), J=21,30)
259          READ (16,4100) (SC1(I,J), J=31,33)
260 140    CONTINUE
261          READ (16,4200) (SR1(I), I=1,10)
262          READ (16,4000) (SR1(I), I=11,18)
263
264      DO 150 I=1,10
265          READ (16,4200) (SC2(I,J), J=1,10)
266          READ (16,4200) (SC2(I,J), J=11,20)
267          READ (16,4200) (SC2(I,J), J=21,30)
268          READ (16,4100) (SC2(I,J), J=31,33)
269 150    CONTINUE
270          READ (16,4200) (SR2(I), I=1,10)
271          READ (16,4000) (SR2(I), I=11,18)
272
273      DO 160 I=1,10
274          READ (16,4200) (SC3(I,J), J=1,10)
275          READ (16,4200) (SC3(I,J), J=11,20)
276          READ (16,4200) (SC3(I,J), J=21,30)
277          READ (16,4100) (SC3(I,J), J=31,33)
278 160    CONTINUE
279          READ (16,4200) (SR3(I), I=1,10)

```

```

280      READ (16,4000) (SR3(I),I=11,18)
281
282      DO 180 I=1,10
283          READ (16,4200) (SC4(I,J),J=1,10)
284          READ (16,4200) (SC4(I,J),J=11,20)
285          READ (16,4200) (SC4(I,J),J=21,30)
286          READ (16,4100) (SC4(I,J),J=31,33)
287 180      CONTINUE
288      READ (16,4200) (SR4(I),I=1,10)
289      READ (16,4000) (SR4(I),I=11,18)
290
291      DO 190 I=1,10
292          READ (16,4200) (SC5(I,J),J=1,10)
293          READ (16,4200) (SC5(I,J),J=11,20)
294          READ (16,4200) (SC5(I,J),J=21,30)
295          READ (16,4100) (SC5(I,J),J=31,33)
296 190      CONTINUE
297      READ (16,4200) (SR5(I),I=1,10)
298      READ (16,4000) (SR5(I),I=11,18)
299
300      DO 200 I=1,10
301          READ (16,4200) (SC6(I,J),J=1,10)
302          READ (16,4200) (SC6(I,J),J=11,20)
303          READ (16,4200) (SC6(I,J),J=21,30)
304          READ (16,4100) (SC6(I,J),J=31,33)
305 200      CONTINUE
306      READ (16,4200) (SR6(I),I=1,10)
307      READ (16,4000) (SR6(I),I=11,18)
308      CLOSE (16)
309
310      OPEN(17,FILE='SDATA',STATUS='OLD')
311      REWIND 17
312      DO 210 I=1,5
313          READ(17,4200) (V(I,J),J=1,10)
314          READ(17,4200) (V(I,J),J=11,20)
315 210      CONTINUE
316      DO 230 K=1,5
317          DO 220 I=1,4
318              READ(17,4300) (SGM(K,I,J),J=1,4)
319 220          CONTINUE
320 230          CONTINUE
321          DO 260 K=1,4
322              DO 250 I=1,4
323                  DO 240 J=1,4
324                      SGM(K,I,J)=SGM(K,I,J)/27.0
325 240                  CONTINUE
326 250              CONTINUE
327 260          CONTINUE
328      CLOSE (17)
329
330
331 4000      FORMAT (8(1X,F6.1))
332 4100      FORMAT (3(1X,F6.1))
333 4200      FORMAT (10(1X,F6.1))
334 4300      FORMAT (4(1X,F6.1))
335

```

```

336      END
337
338
339 *****
340
341 * RENUMBERS THE GRID - SINCE MESH IS NUMBERED DIFFERENTLY
342 * FOR EACH FIT (LINEAR, QUADRATIC, AND CUBIC) ALLOWS THE DATA
343 * FILE 'MESH' TO REMAIN SIMPLE, AND BE USED BY ALL THREE
344 * CODES - NUMBERING IS AS PER FIGURE 2-4
345
346      SUBROUTINE CHGRID (PTNODE, CORDND, N, NTRIA)
347
348      PARAMETER (MNODE=151, MNTRIA=50)
349
350      DOUBLE PRECISION CORDND(MNODE,2), D,E
351      DOUBLE PRECISION ML(MNTRIA,10,10)
352      DOUBLE PRECISION NL(MNTRIA,16,10,10), NLI(MNTRIA,4,10)
353      DOUBLE PRECISION MG(MNODE,MNODE)
354      DOUBLE PRECISION GT(MNTRIA,10,10), LI(MNTRIA,10,4)
355      INTEGER N, NTRIA, TRI, A,B,C
356      INTEGER PTNODE(MNTRIA,11)
357      COMMON MG, ML, NL, NLI, LI, GT
358
359
360      DO 100 I=1, NTRIA
361          K=(3*N)+I
362          CORDND(K,1)=(1.0/3.0)*(CORDND(PTNODE(I,1),1) + CORDND(
363      C      PTNODE(I,2),1) + CORDND(PTNODE(I,3),1))
364          CORDND(K,2)=(1.0/3.0)*(CORDND(PTNODE(I,1),2) + CORDND(
365      C      PTNODE(I,2),2) + CORDND(PTNODE(I,3),2))
366 100      CONTINUE
367
368
369
370      DO 110 TRI=1, NTRIA
371          A=PTNODE(TRI,1)
372          B=PTNODE(TRI,2)
373          C=PTNODE(TRI,3)
374          PTNODE(TRI,11)=PTNODE(TRI,4)
375          PTNODE(TRI,1)=3*A-2
376          PTNODE(TRI,2)=3*A-1
377          PTNODE(TRI,3)=3*A
378          PTNODE(TRI,4)=3*B-2
379          PTNODE(TRI,5)=3*B-1
380          PTNODE(TRI,6)=3*B
381          PTNODE(TRI,7)=3*C-2
382          PTNODE(TRI,8)=3*C-1
383          PTNODE(TRI,9)=3*C
384          PTNODE(TRI,10)=3*N+TRI
385 110      CONTINUE
386
387
388      DO 120 I=N, 1, -1
389          D=CORDND(I,1)
390          E=CORDND(I,2)
391          K=3*I-2

```

```

392     CORDND(K,1)=D
393     CORDND(K,2)=E
394     CORDND(K+1,1)=D
395     CORDND(K+1,2)=E
396     CORDND(K+2,1)=D
397     CORDND(K+2,2)=E
398 120     CONTINUE
399
400     N=3*N + NTRIA
401
402
403
404     END
405
406
407
408
409 *****
410
411 * FIND THE MATRIX GT, OF (2-34)
412
413     SUBROUTINE INFCN(TRI,G1,G2,G3,F1,F2,F3)
414
415     PARAMETER (MNODE=151 , MNTRIA=50)
416     DOUBLE PRECISION GT(MNTRIA,10,10),LI(MNTRIA,10,4)
417     DOUBLE PRECISION G1,G2,G3,F1,F2,F3,F
418     DOUBLE PRECISION ML(MNTRIA,10,10)
419     DOUBLE PRECISION NLM(MNTRIA,16,10,10),NLI(MNTRIA,4,10)
420     DOUBLE PRECISION MG(MNODE,MNODE)
421     INTEGER TRI
422     COMMON MG,ML,NLM,NLI,LI,GT
423
424     DO 550 I=1,10
425         DO 500 J=1,10
426             GT(TRI,I,J)=0.0
427 500         CONTINUE
428 550     CONTINUE
429
430     F=G2*F3-G3*F2
431     GT(TRI,1,1)=1.0
432     GT(TRI,2,1)=3*(G3*F1-G1*F3)/F
433     GT(TRI,2,2)=F3/F
434     GT(TRI,2,3)=-G3/F
435     GT(TRI,3,1)=3*(G1*F2-G2*F1)/F
436     GT(TRI,3,2)=-F2/F
437     GT(TRI,3,3)=G2/F
438
439     F=G3*F1-G1*F3
440     GT(TRI,4,4)=1.0
441     GT(TRI,5,4)=3*(G1*F2-G2*F1)/F
442     GT(TRI,5,5)=F1/F
443     GT(TRI,5,6)=-G1/F
444     GT(TRI,6,4)=3*(G2*F3-G3*F2)/F
445     GT(TRI,6,5)=-F3/F
446     GT(TRI,6,6)=G3/F
447

```

```

448      F=G1*F2-G2*F1
449      GT(TRI,7,7)=1.0
450      GT(TRI,8,7)=3*(G2*F3-G3*F2)/F
451      GT(TRI,8,8)=F2/F
452      GT(TRI,8,9)=-G2/F
453      GT(TRI,9,7)=3*(G3*F1-G1*F3)/F
454      GT(TRI,9,8)=-F1/F
455      GT(TRI,9,9)=G1/F
456
457      GT(TRI,10,10)=27.0
458
459      DO 130 I=1,7,3
460          DO 120 J=I,I+2
461              GT(TRI,10,I)=GT(TRI,10,I)-GT(TRI,J,I)
462              GT(TRI,10,I+1)=GT(TRI,10,I+1)-GT(TRI,J,I+1)
463              GT(TRI,10,I+2)=GT(TRI,10,I+2)-GT(TRI,J,I+2)
464 120      CONTINUE
465 130      CONTINUE
466
467      END
468
469
470 *****
471
472 * BOUNDARY MATRIX - ASSEMBLAGE EXPLAINED IN APPENDIX C
473
474      SUBROUTINE BNDRY (U1,U2,U3,G1,G2,G3,BC1,BC2,BC3,BR1
475 C      ,BR2,BR3,SIGMAT,MB,D,AREAS,TRI)
476
477      PARAMETER (MNODE=151 , MNTRIA=50)
478      DOUBLE PRECISION U1,U2,U3,G1,G2,G3,F
479      DOUBLE PRECISION BC1(10,20),BC2(10,20),BC3(10,20)
480      DOUBLE PRECISION BC(10,20)
481      DOUBLE PRECISION BR1(10),BR2(10),BR3(10),BR(10)
482      DOUBLE PRECISION MB(10,10),D(10,2),SIGMAT,AREAS(MNTRIA)
483      DOUBLE PRECISION ML(MNTRIA,10,10)
484      DOUBLE PRECISION NLM(MNTRIA,16,10,10),NLI(MNTRIA,4,10)
485      DOUBLE PRECISION MG(MNODE,MNODE)
486      DOUBLE PRECISION GT(MNTRIA,10,10),LI(MNTRIA,10,4)
487      INTEGER TRI
488      COMMON MG,ML,NLM,NLI,LI,GT
489
490 * ASSEMBLE THE DERIVATIVE MATRIX, TO BE OVERLAYED
491 * NOTE - PASSED AS DRVS
492      D(1,1)=G1
493      D(2,1)=G1
494      D(3,1)=G1
495      D(4,1)=G2
496      D(5,1)=G2
497      D(6,1)=G2
498      D(7,1)=G3
499      D(8,1)=G3
500      D(9,1)=G3
501      D(10,1)=G1
502      D(1,2)=0.0
503      D(2,2)=G2

```

```

504      D(3,2)=G3
505      D(4,2)=0.0
506      D(5,2)=G3
507      D(6,2)=G1
508      D(7,2)=0.0
509      D(8,2)=G1
510      D(9,2)=G2
511      D(10,2)=G2
512
513 * MULTIPLY THE COEFFICIENT MATRICES AND ROWS BY APPROPRIATE
514 * U VALUE - THEN SUM
515      F=SIGMAT*4.0*AREAS(TRI)/40320.0
516      DO 100 I=1,10
517          BR(I)=(U1*BR1(I)+U2*BR2(I)+U3*BR3(I))*F
518          DO 50 J=1,20
519              BC(I,J)=(U1*BC1(I,J)+U2*BC2(I,J)+U3*BC3(I,J))*F
520 50      CONTINUE
521 100      CONTINUE
522
523 * OVERLAY THE DERIVATIVE MATRIX TO FORM MB
524      DO 250 I=1,10
525          DO 200 J=1,10
526              MB(I,J)=BC(I,(2*J)-1)*D(I,1)+BC(I,2*J)*D(I,2)
527 200      CONTINUE
528 250      CONTINUE
529
530 * AUGMENT THE LAST ROW
531      DO 300 I=1,10
532          MB(10,I)=MB(10,I)+G3*BR(I)
533 300      CONTINUE
534
535 * PLACE IN ITS QUADRATIC FORM
536      DO 400 I=1,10
537          DO 350 J=1,I
538              MB(I,J)=(MB(I,J)+MB(J,I))/2.0
539              MB(J,I)=MB(I,J)
540 350      CONTINUE
541 400      CONTINUE
542
543      END
544
545
546 *****
547
548 * STREAMING MATRIX - ASSEMBLAGE EXPLAINED IN APPENDIX D
549
550      SUBROUTINE STREAM (SC1,SR1,SC2,SR2,SC3,SR3,SC4,SR4,SC5,SR5,
551      C                      SC6,SR6,MS,U1,U2,U3,G1,G2,G3,AREAS,TRI,
552      C                      DRVS)
553
554      PARAMETER (MNODE=151 , MNTRIA=50)
555
556      DOUBLE PRECISION AREAS(MNTRIA)
557      DOUBLE PRECISION SC1(10,33),SR1(18),SC2(10,33),SR2(18)
558      DOUBLE PRECISION SC3(10,33),SR3(18),SC4(10,33),SR4(18)
559      DOUBLE PRECISION SC5(10,33),SR5(18),SC6(10,33),SR6(18)

```

```

560      DOUBLE PRECISION  GG(3),DS(10,33),SC(10,33),A,B,C,D,E,F,G
561      DOUBLE PRECISION  SR(18),DR(18)
562      DOUBLE PRECISION  MS(10,10),DRVS(10,2)
563      DOUBLE PRECISION  G1,G2,G3,U1,U2,U3
564      DOUBLE PRECISION  ML(MNTRIA,10,10)
565      DOUBLE PRECISION  NLM(MNTRIA,16,10,10),NLI(MNTRIA,4,10)
566      DOUBLE PRECISION  MG(MNODE,MNODE)
567      DOUBLE PRECISION  GT(MNTRIA,10,10),LI(MNTRIA,10,4)
568      INTEGER TRI
569      COMMON MG,ML,NLM,NLI,LI,GT
570
571 * ASSEMBLE THE MATRIX OF DERIVATIVES
572      GG(1)=G1
573      GG(2)=G2
574      GG(3)=G3
575
576 * FILL IN COLUMNS 1,2,3,12,13,14,23,24,25 OF DS
577      DO 110 I=1,7,3
578          L=1+(I-1)/3
579          K=1+((I-1)*11/3)
580          DO 100 J=1,10
581              DS(J,K)=DRVS(J,1)*GG(L)
582              DS(J,K+1)=DRVS(J,2)*GG(L)
583              DS(J,K+2)=0.0
584 100      CONTINUE
585 110      CONTINUE
586
587      DS(10,3)=G1*G3
588      DS(10,14)=G2*G3
589      DS(10,25)=G3*G3
590
591 * FILL IN REMAINING COLUMNS
592      DO 120 J=1,10
593          DS(J,4)=DRVS(J,1)*G1
594          DS(J,5)=DRVS(J,2)*G1
595          DS(J,6)=DRVS(J,1)*G2
596          DS(J,7)=DRVS(J,2)*G2
597          DS(J,8)=DS(J,4)
598          DS(J,9)=DS(J,5)
599          DS(J,10)=DRVS(J,1)*G3
600          DS(J,11)=DRVS(J,2)*G3
601          DS(J,15)=DS(J,6)
602          DS(J,16)=DS(J,7)
603          DS(J,17)=DS(J,10)
604          DS(J,18)=DS(J,11)
605          DS(J,19)=DS(J,6)
606          DS(J,20)=DS(J,7)
607          DS(J,21)=DS(J,4)
608          DS(J,22)=DS(J,5)
609          DS(J,26)=DS(J,10)
610          DS(J,27)=DS(J,11)
611          DS(J,28)=DS(J,4)
612          DS(J,29)=DS(J,5)
613          DS(J,30)=DS(J,10)
614          DS(J,31)=DS(J,11)
615          DS(J,32)=DS(J,6)

```

```

616          DS(J,33)=DS(J,7)
617 120      CONTINUE
618
619          DS(10,6)=G1*G3
620          DS(10,7)=0.0
621          DS(10,10)=G1*G3
622          DS(10,11)=0.0
623          DS(10,17)=G2*G3
624          DS(10,18)=0.0
625          DS(10,21)=G2*G3
626          DS(10,22)=0.0
627          DS(10,28)=G3*G3
628          DS(10,29)=0.0
629          DS(10,32)=G3*G3
630          DS(10,33)=0.0
631
632          DR(1)=G2*G2
633          DR(2)=G2*G3
634          DR(3)=DR(2)
635          DR(4)=G3*G3
636          DR(5)=G1*G3
637          DR(6)=DR(4)
638          DR(7)=G1*G1
639          DR(8)=DR(5)
640          DR(9)=DR(7)
641          DR(10)=G1*G2
642          DR(11)=DR(10)
643          DR(12)=DR(1)
644          DR(13)=DR(7)
645          DR(14)=DR(10)
646          DR(15)=DR(5)
647          DR(16)=DR(1)
648          DR(17)=DR(2)
649          DR(18)=DR(4)
650
651 * MULTIPLY THE COEFICIENT MATRICES AND ROWS BY THE
652 * APPROPRIATE U'S - THEN SUM
653          A=U1*U1
654          B=U2*U2
655          C=U3*U3
656          D=U1*U2*2.0
657          E=U2*U3*2.0
658          F=U1*U3*2.0
659          G=2.0*AREAS(TRI)/40320.0
660          DO 140 I=1,10
661              DO 130 J=1,33
662                  SC(I,J)=(SC1(I,J)*A + SC2(I,J)*B + SC3(I,J)*C +
663                      C          SC4(I,J)*D + SC5(I,J)*E + SC6(I,J)*F)*G
664 130          CONTINUE
665 140          CONTINUE
666          DO 150 I=1,18
667              SR(I)=(SR1(I)*A + SR2(I)*B + SR3(I)*C +
668                  C          SR4(I)*D + SR5(I)*E + SR6(I)*F)*G
669 150          CONTINUE
670
671 * COMPUTE COLUMNS 1,4,7 OF STREAMING MATRIX

```

```

672      DO 170 I=1,10
673          DO 160 J=1,7,3
674              K=1 + ((J-1)*11/3)
675              MS(I,J)=SC(I,K)*DS(I,K) + SC(I,K+1)*DS(I,K+1)
676              C          + SC(I,K+2)*DS(I,K+2)
677 160      CONTINUE
678 170      CONTINUE
679
680 * COLUMNS 2,5, AND 8
681      DO 190 I=1,10
682          DO 180 J=2,8,3
683              K=4+((J-2)*11/3)
684              MS(I,J)=SC(I,K)*DS(I,K) + SC(I,K+1)*DS(I,K+1)
685              C          + SC(I,K+2)*DS(I,K+2) + SC(I,K+3)*DS(I,K+3)
686              K=K+4
687              MS(I,J+1)=SC(I,K)*DS(I,K) + SC(I,K+1)*DS(I,K+1)
688              C          + SC(I,K+2)*DS(I,K+2) + SC(I,K+3)*DS(I,K+3)
689 180      CONTINUE
690 190      CONTINUE
691 * AUGMENT THE LAST ROW
692      DO 200 I=2,8,3
693          K=1 + 4*(I-2)/3
694          MS(10,I)=MS(10,I)+SR(K)*DR(K)+SR(K+1)*DR(K+1)
695          MS(10,I+1)=MS(10,I+1)+SR(K+2)*DR(K+2)+SR(K+3)*DR(K+3)
696 200      CONTINUE
697
698      MS(10,10)=0.0
699      DO 210 I=13,18
700          MS(10,10)=MS(10,10)+SR(I)*DR(I)
701 210      CONTINUE
702
703 * FORM COLUMN 10 WITH SYMMETRY
704      DO 220 I=1,9
705          MS(I,10)=MS(10,I)
706 220      CONTINUE
707
708      END
709
710
711 *****
712
713 * LOCAL MATRIX - MULTIPLY ABSORBING, BOUNDARY AND STREAMING
714 * BY APPROPRIATE CONSTANTS - AND SUM
715 * PRE AND POST MULTIPLY BY GT TO COMPLETELY PREPARE FOR
716 * GLOBAL ASSEMBLAGE
717
718      SUBROUTINE LMATRX(MA,MB,MS,AREAS,SIGMAT,TRI)
719
720      PARAMETER (MNODE=151 , MNTRIA=50)
721      DOUBLE PRECISION AREAS(MNTRIA),MA(10,10)
722      DOUBLE PRECISION MB(10,10),MS(10,10),MT(10,10)
723      DOUBLE PRECISION SIGMAT,F
724      DOUBLE PRECISION ML(MNTRIA,10,10)
725      DOUBLE PRECISION NLM(MNTRIA,16,10,10),NLI(MNTRIA,4,10)
726      DOUBLE PRECISION MG(MNODE,MNODE)
727      DOUBLE PRECISION GT(MNTRIA,10,10),LI(MNTRIA,10,4)

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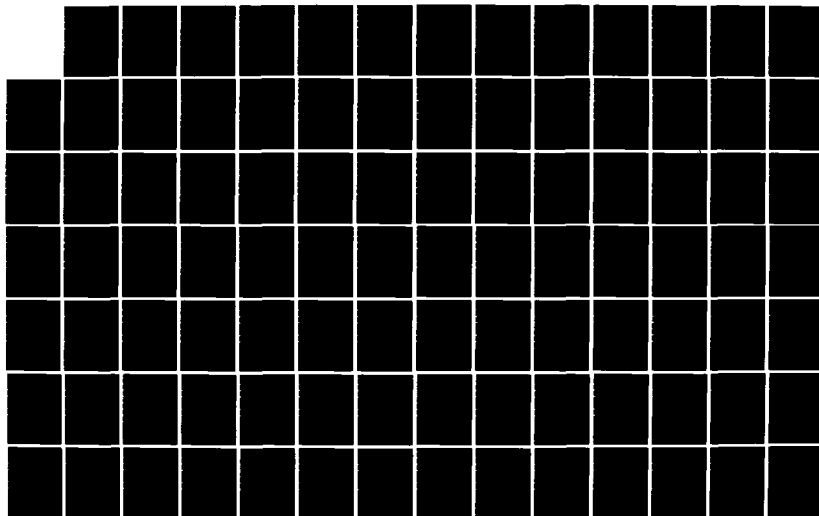
A FINITE ELEMENT SOLUTION OF THE TRANSPORT EQUATION(U)  
AIR FORCE INST OF TECH WRIGHT-PATTERSON AFB OH SCHOOL  
OF ENGINEERING F A TARANTINO MAR 85 AFIT/GNE/PH/85M-19

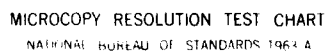
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MICROCOPY RESOLUTION TEST CHART  
NATIONAL BUREAU OF STANDARDS 1963-A

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728      INTEGER TRI
729      COMMON MG,ML,NLM,NLI,LI,GT
730
731      F=SIGMAT*SIGMAT*2.0*AREAS(TRI)/40320.0
732
733
734      DO 830 I=1,10
735          DO 820 J=1,10
736              ML(TRI,J,I)=MB(J,I) + MA(J,I)*F + MS(J,I)
737 820          CONTINUE
738 830          CONTINUE
739
740      DO 860 I=1,10
741          DO 850 J=1,10
742              MT(I,J)=0.0
743              DO 840 K=1,10
744                  MT(I,J)=MT(I,J) + GT(TRI,K,I)*ML(TRI,K,J)
745 840          CONTINUE
746 850          CONTINUE
747 860          CONTINUE
748      DO 890 I=1,10
749          DO 880 J=1,10
750              ML(TRI,I,J)=0.0
751              DO 870 K=1,10
752                  ML(TRI,I,J)=ML(TRI,I,J) + MT(I,K)*GT(TRI,K,J)
753 870          CONTINUE
754 880          CONTINUE
755 890          CONTINUE
756
757      END
758
759
760      *****
761
762      * ASSEMBLE LOCAL TERMS GLOBALLY
763
764      SUBROUTINE ASEMBL(PTNODE,TRI)
765
766      PARAMETER (MNODE=151 , MNTRIA=50)
767
768      DOUBLE PRECISION ML(MNTRIA,10,10)
769      DOUBLE PRECISION NLM(MNTRIA,16,10,10),NLI(MNTRIA,4,10)
770      DOUBLE PRECISION MG(MNODE,MNODE)
771      DOUBLE PRECISION GT(MNTRIA,10,10),LI(MNTRIA,10,4)
772      INTEGER PTNODE(MNTRIA,11),TRI,R(10)
773      COMMON MG,ML,NLM,NLI,LI,GT
774
775      DO 900 I=1,10
776          R(I)=PTNODE(TRI,I)
777 900      CONTINUE
778
779      DO 920 I=1,10
780          DO 910 J=1,10
781              MG(R(I),R(J))=MG(R(I),R(J)) + ML(TRI,I,J)
782 910          CONTINUE
783 920          CONTINUE

```

```

784
785     END
786
787
788 *****
789
790 * INSURE FLUXES (AND IN THIS CASE U-CURRENTS) ARE AS SPECIFIED
791 * ON BOUNDARIES - IF FLUXES ONLY ARE TO BE SPECIFIED DELETE
792 * THE I+2 TERMS MODIFICATION
793
794     SUBROUTINE BNDEND(CORDND,PHI,N,NTRIA,RANGE)
795
796     PARAMETER (MNODE=151 , MNTRIA=50)
797
798     DOUBLE PRECISION  CORDND(MNODE,2),PHI(MNODE)
799     DOUBLE PRECISION  ML(MNTRIA,10,10)
800     DOUBLE PRECISION  NLM(MNTRIA,16,10,10),NLI(MNTRIA,4,10)
801     DOUBLE PRECISION  MG(MNODE,MNODE)
802     DOUBLE PRECISION  GT(MNTRIA,10,10),LI(MNTRIA,10,4)
803     DOUBLE PRECISION  RANGE
804     INTEGER N,NTRIA
805     COMMON MG,ML,NLM,NLI,LI,GT
806
807     DO 120 I=1,N-NTRIA,3
808         IF (CORDND(I,1).EQ.0.0.AND.CORDND(I,2).GE.0.0) THEN
809             MG(I,I)=MG(I,I)*1.0E+20
810             PHI(I)=PHI(I)*MG(I,I)
811             MG(I+2,I+2)=MG(I+2,I+2)*1.0E+20
812             PHI(I+2)=PHI(I+2)*MG(I+2,I+2)
813         ELSE
814             IF (CORDND(I,1).EQ.RANGE.AND.CORDND(I,2).LE.0.0) THEN
815                 MG(I,I)=MG(I,I)*1.0E+20
816                 PHI(I)=PHI(I)*MG(I,I)
817                 MG(I+2,I+2)=MG(I+2,I+2)*1.0E+20
818                 PHI(I+2)=PHI(I+2)*MG(I+2,I+2)
819             ENDIF
820         ENDIF
821     120 CONTINUE
822
823     END
824
825
826 *****
827
828 * CALCULATE VALUE OF VARIATIONAL INTEGRAL OVER AN ELEMENT
829
830     SUBROUTINE PENLTY(PHI,PTNODE,PEN,NTRIA,COLUMN)
831
832     PARAMETER (MNODE=151 , MNTRIA=50)
833     DOUBLE PRECISION  ML(MNTRIA,10,10),PHI(MNODE),PEN(MNTRIA)
834     DOUBLE PRECISION  P(10),L(10)
835     DOUBLE PRECISION  S(10),F
836     DOUBLE PRECISION  NLM(MNTRIA,16,10,10),NLI(MNTRIA,4,10)
837     DOUBLE PRECISION  MG(MNODE,MNODE)
838     DOUBLE PRECISION  GT(MNTRIA,10,10),LI(MNTRIA,10,4)
839     INTEGER TRI,NTRIA,PTNODE(MNTRIA,11)

```

```

840     INTEGER TRIP,COLUMN(32,2)
841     COMMON MG,ML,NLM,NLI,LI,GT
842
843     DO 100 TRI=1,NTRIA
844 * LOCAL MATRIX CONTRIBUTION
845     DO 20 I=1,10
846         P(I)=PHI(PTNODE(TRI,I))
847     20 CONTINUE
848     DO 40 I=1,10
849         L(I)=0.0
850         DO 30 J=1,10
851             L(I)=L(I) + ML(TRI,I,J)*P(J)
852     30 CONTINUE
853     40 CONTINUE
854     PEN(TRI)=0.0
855     DO 50 I=1,10
856         PEN(TRI)=PEN(TRI) + L(I)*P(I)
857     50 CONTINUE
858 * SUM OF NON LOCAL MATRICES CONTRIBUTIONS
859     K=COLUMN(PTNODE(TRI,11),1)
860     DO 70 TRIP=K,K-1+COLUMN(PTNODE(TRI,11),2)
861         DO 55 I=1,10
862             S(I)=PHI(PTNODE(TRIP,I))
863     55 CONTINUE
864         DO 65 I=1,10
865             L(I)=0.0
866             DO 60 J=1,10
867                 L(I)=L(I) + NLM(TRI,TRIP,I,J)*S(J)
868     60 CONTINUE
869     65 CONTINUE
870         DO 68 I=1,10
871             PEN(TRI)=PEN(TRI)+L(I)*P(I)
872     68 CONTINUE
873     70 CONTINUE
874     PEN(TRI)=.5*PEN(TRI)
875 100 CONTINUE
876
877     END
878
879 *****
880
881 * PRINT OUTPUT - COMPARE FE SOLUTION WITH Pn OR ANALYTICAL
882 * IF NO SCATTER
883
884     SUBROUTINE OUTPUT(PHI,N,PTNODE,CORDND,NTRIA,
885 C                     CHECK1,PEN,SIGMAS,RANGE,SIGMAT)
886
887     PARAMETER (MNODE=151 , MNTRIA=50)
888     DOUBLE PRECISION PHI(MNODE),CORDND(MNODE,2)
889     DOUBLE PRECISION PEN(MNTRIA),PENTOT
890     DOUBLE PRECISION ML(MNTRIA,10,10)
891     DOUBLE PRECISION NLM(MNTRIA,16,10,10),NLI(MNTRIA,4,10)
892     DOUBLE PRECISION MG(MNODE,MNODE)
893     DOUBLE PRECISION GT(MNTRIA,10,10),LI(MNTRIA,10,4)
894     DOUBLE PRECISION RANGE,SIGMAT,TPEN
895     INTEGER PTNODE(MNTRIA,11),TRI,N,NTRIA

```

```

896 LOGICAL CHECK1
897 COMMON MG,ML,NLM,NLI,LI,GT
898
899 IF (CHECK1) THEN
900
901 PRINT*, 'NTRIA      N      SIGMAS'
902 WRITE (*,4999) NTRIA,N,SIGMAS
903 4999 FORMAT (3X,I3,5X,I3,5X,F6.3)
904 PRINT*, 'RANGE IS....',RANGE
905
906 PRINT*, 'NODAL VALUES OF THE FLUX'
907 J=N-NTRIA
908 DO 100 I=1,J,6
909     K=1+(I-1)/3
910     WRITE(*,6010) K,PHI(I),K+1,PHI(I+3)
911 6010 FORMAT(2(2X,I3,3X,F9.4))
912 100 CONTINUE
913
914 PRINT*, 'ELEMENT PENALTY VALUES'
915 PENTOT=0.0
916 TPEN=0.0
917 DO 110 I=1,NTRIA,2
918     WRITE(*,6221) I,PEN(I),I+1,PEN(I+1)
919     PENTOT=PENTOT + ABS(PEN(I)) + ABS(PEN(I+1))
920     TPEN=TPEN + PEN(I) + PEN(I+1)
921 110 CONTINUE
922 PRINT*, 'TOTAL PENALTY .... AND SUM OF ABS(PENALTY) ARE ..'
923 WRITE(*,6222) TPEN,PENTOT
924 6221 FORMAT (2(2X,I3,5X,E11.5))
925 6222 FORMAT (2(10X,E11.5))
926
927 * COMPARE FE SOLUTION WITH APPROPRIATE BENCHMARK
928 IF (SIGMAS.EQ.0.0) THEN
929     CALL ANALY(PHI,CORDND,SIGMAT,N,NTRIA,RANGE)
930 ELSE
931     CALL PN(PHI,CORDND,SIGMAS,N,NTRIA,RANGE)
932 ENDIF
933
934 ELSE
935 * IF DESIRED TURN ON DIAGNOSTIC OUTPUT HERE
936 GO TO 301
937 PRINT*, 'MESH DEFINITION'
938 PRINT*, ' TRIANGLE      GLOBAL NODES'
939 DO 50 TRI=1,NTRIA
940     WRITE(*,6050) TRI,(PTNODE(TRI,I),I=1,7,3)
941 6050 FORMAT(4X,I3,8X,3(I3,3X))
942 50 CONTINUE
943
944 PRINT*
945 PRINT*, '      NODE      COORDINATES (X,U)'
946 DO 60 I=1,N-NTRIA,3
947     K=(I+2)/3
948     WRITE(*,6060) K,(CORDND(I,J),J=1,2)
949 6060 FORMAT(4X,I3,7X,2(F7.3,3X))
950 60 CONTINUE
951

```

```

952      PRINT*
953      PRINT*, 'GLOBAL MATRIX'
954      PRINT*
955      DO 300 I=1,N
956          WRITE(*,6210) (MG(I,J),J=1,N)
957 6210      FORMAT(1X,":",16(1X,F6.3))
958          WRITE(*,6220)
959 6220      FORMAT(1X,":")
960 300      CONTINUE
961 301      ENDIF
962
963 350      END
964
965 *****
966
967 * ASSEMBLE SCATTERING MATRICES (NON LOCAL) - A SEPARATE
968 * SUBROUTINE IS USED BECAUSE DIMENSIONS OF NLM ARE DIFFERENT
969 * THAN ML
970
971      SUBROUTINE SASMBL(PTNODE,TRI,TRIP)
972
973      PARAMETER (MNODE=151 , MNTRIA=50)
974      DOUBLE PRECISION ML(MNTRIA,10,10)
975      DOUBLE PRECISION NLM(MNTRIA,16,10,10),NLI(MNTRIA,4,10)
976      DOUBLE PRECISION MG(MNODE,MNODE)
977      DOUBLE PRECISION GT(MNTRIA,10,10),LI(MNTRIA,10,4)
978      INTEGER PTNODE(MNTRIA,11),TRI,R(10),TRIP
979      INTEGER L(10)
980      COMMON MG,ML,NLM,NLI,LI,GT
981
982      DO 900 I=1,10
983          R(I)=PTNODE(TRI,I)
984          L(I)=PTNODE(TRIP,I)
985 900      CONTINUE
986
987      DO 920 I=1,10
988          DO 910 J=1,10
989              MG(R(I),L(J))=MG(R(I),L(J)) + NLM(TRI,TRIP,I,J)
990 910          CONTINUE
991 920      CONTINUE
992      END
993
994
995
996 *****
997
998 * COMPARE FE SOLUTION TO ANALYTICAL IN THE CASE OF NO SCATTER
999
1000      SUBROUTINE ANALY(PHI,CORDND,SIGMAT,N,NTRIA,RANGE)
1001
1002      PARAMETER (MNODE=151 , MNTRIA=50)
1003      DOUBLE PRECISION CORDND(MNODE,2),PHI(MNODE),A,RANGE
1004      DOUBLE PRECISION PERC,TPERC
1005      DOUBLE PRECISION ML(MNTRIA,10,10)
1006      DOUBLE PRECISION NLM(MNTRIA,16,10,10),NLI(MNTRIA,4,10)
1007      DOUBLE PRECISION MG(MNODE,MNODE)

```

```

1008 DOUBLE PRECISION GT(MNTRIA,10,10),LI(MNTRIA,10,4)
1009 INTEGER N,NTRIA
1010 COMMON MG,ML,NLM,NLI,LI,GT
1011
1012 TPERC=0.0
1013 K=0
1014 PRINT*, ' COORDINATES      CURRENTS      FIN ELEM'
1015 PRINT*, '      X      U      X      U      FLUX      FLUX      % DIFF'
1016 DO 100 I=1,N-NTRIA,3
1017     IF (CORDND(I,2).GT.0.0) THEN
1018         A=CORDND(I,2)*EXP(-SIGMAT/CORDND(I,2)*CORDND(I,1))
1019         PERC=100*ABS(PHI(I)-A)/A
1020         WRITE(*,5002) CORDND(I,1),CORDND(I,2),PHI(I+1),PHI(I+2)
1021         C      ,PHI(I),A,PERC
1022         TPERC=TPERC+PERC
1023         IF (CORDND(I,1).NE.0.0.AND.CORDND(I,1).NE.RANGE) THEN
1024             K=K+1
1025         ENDIF
1026     ENDIF
1027 100 CONTINUE
1028 PRINT*, 'AVERAGE % DIFFERENCE IS ..',TPERC/K
1029 D=NTRIA*.5/RANGE
1030 PRINT*, 'FOR AN AVG. OF',D,' TRIANGLES PER MFP FOR U>0 '
1031
1032 5002 FORMAT(6(2X,F6.3),2X,F6.2)
1033
1034 END
1035 *****
1036
1037 * CALCULATE THE NON LOCAL MATRIX FOR TRIANGLE TRI
1038 * INTO TRIANGLE TRIP
1039
1040 SUBROUTINE NLMTRX(TRI,TRIP,SIGMAS,SIGMAT,
1041 C      TIME,V6,SA,SB)
1042
1043     PARAMETER (MNODE=151 , MNTRIA=50)
1044     DOUBLE PRECISION ML(MNTRIA,10,10)
1045     DOUBLE PRECISION NLM(MNTRIA,16,10,10),NLI(MNTRIA,4,10)
1046     DOUBLE PRECISION MG(MNODE,MNODE)
1047     DOUBLE PRECISION GT(MNTRIA,10,10),LI(MNTRIA,10,4)
1048     DOUBLE PRECISION SIGMAS,SIGMAT,SA(10,10),SB(10,10)
1049     DOUBLE PRECISION V6
1050     INTEGER TRI,TRIP,TIME
1051     COMMON MG,ML,NLM,NLI,LI,GT
1052
1053 * CALCULATE CONSTANTS
1054     A=.5*SIGMAS*SIGMAS - SIGMAS*SIGMAT
1055     B=-SIGMAS
1056     F=V6*A/720.0
1057     G=V6*B/5040.0
1058
1059 * ZERO THE NON LOCAL MATRIX
1060     IF (TIME.EQ.1) THEN
1061         DO 50 I=1,3
1062             DO 40 J=1,3
1063                 NLM(TRI,TRIP,I,J)=0.0

```

```

1064 40          CONTINUE
1065 50          CONTINUE
1066          ENDIF
1067
1068 * CALCULATE THE NON LOCAL MATRIX
1069          DO 100 I=1,10
1070              DO 60 J=1,10
1071                  NLN(TRI,TRIP,I,J)=NLN(TRI,TRIP,I,J)+(F*SA(I,J)
1072                  C      +G*SB(I,J))
1073 60          CONTINUE
1074 100          CONTINUE
1075
1076          END
1077 *****
1078 * FIND PHI OF (L1,L2,L3) FOR THE TRIANGLE IN QUESTION
1079
1080          SUBROUTINE PHII(TRI,L1,L2,L3,D)
1081
1082          PARAMETER (MNODE=151 , MNTRIA=50)
1083          DOUBLE PRECISION L1,L2,L3,D(10),W(10)
1084          DOUBLE PRECISION ML(MNTRIA,10,10)
1085          DOUBLE PRECISION NLN(MNTRIA,16,10,10),NLI(MNTRIA,4,10)
1086          DOUBLE PRECISION MG(MNODE,MNODE)
1087          DOUBLE PRECISION GT(MNTRIA,10,10),LI(MNTRIA,10,4)
1088          INTEGER TRI
1089          COMMON MG,ML,NLN,NLI,LI,GT
1090
1091          W(1)=L1**3
1092          W(2)=L2*L1**2
1093          W(3)=L3*L1**2
1094          W(4)=L2**3
1095          W(5)=L3*L2**2
1096          W(6)=L1*L2**2
1097          W(7)=L3**3
1098          W(8)=L1*L3**2
1099          W(9)=L2*L3**2
1100          W(10)=L1*L2*L3
1101          DO 30 I=1,10
1102              D(I)=0.0
1103              DO 20 J=1,10
1104                  D(I)=D(I)+W(J)*GT(TRI,J,I)
1105 20          CONTINUE
1106 30          CONTINUE
1107
1108          END
1109 *****
1110
1111 * FIND D(PHI)/DX FOR THE TRIANGLE UNDER SCRUTINY
1112
1113          SUBROUTINE PHIX(TRI,L1,L2,L3,G1,G2,G3,DX)
1114
1115          PARAMETER (MNODE=151 , MNTRIA=50)
1116          DOUBLE PRECISION L1,L2,L3,G1,G2,G3,W(10),DX(10)
1117          DOUBLE PRECISION ML(MNTRIA,10,10)
1118          DOUBLE PRECISION NLN(MNTRIA,16,10,10),NLI(MNTRIA,4,10)
1119          DOUBLE PRECISION MG(MNODE,MNODE)

```

```

1120      DOUBLE PRECISION GT(MNTRIA,10,10),LI(MNTRIA,10,4)
1121      INTEGER TRI
1122      COMMON MG,ML,NLM,NLI,LI,GT
1123
1124
1125
1126 * FIND D(PHI)/DX
1127      W(1)=3.0*G1*L1**2
1128      W(2)=G2*L1**2+L2*G1*2.0*L1
1129      W(3)=G3*L1**2+L3*G1*2.0*L1
1130      W(4)=3.0*G2*L2**2
1131      W(5)=G3*L2**2+L3*G2*2.0*L2
1132      W(6)=G1*L2**2+L1*G2*2.0*L2
1133      W(7)=3.0*G3*L3**2
1134      W(8)=G1*L3**2+L1*G3*2.0*L3
1135      W(9)=G2*L3**2+L2*G3*2.0*L3
1136      W(10)=G1*L2*L3+G2*L1*L3+G3*L1*L2
1137      DO 50 I=1,10
1138          DX(I)=0.0
1139          DO 40 J=1,10
1140              DX(I)=DX(I)+W(J)*GT(TRI,J,I)
1141 40      CONTINUE
1142 50      CONTINUE
1143
1144      END
1145 *****
1146 * FIND D(PHI)**2/DX**2
1147
1148      SUBROUTINE PHIXX(TRI,L1,L2,L3,G1,G2,G3,DXX)
1149
1150      PARAMETER (MNODE=151 , MNTRIA=50)
1151      DOUBLE PRECISION L1,L2,L3,G1,G2,G3,W(10),DXX(10)
1152      DOUBLE PRECISION ML(MNTRIA,10,10)
1153      DOUBLE PRECISION NLM(MNTRIA,16,10,10),NLI(MNTRIA,4,10)
1154      DOUBLE PRECISION MG(MNODE,MNODE)
1155      DOUBLE PRECISION GT(MNTRIA,10,10),LI(MNTRIA,10,4)
1156      INTEGER TRI
1157      COMMON MG,ML,NLM,NLI,LI,GT
1158
1159      W(1)=6.0*L1*G1**2
1160      W(2)=4.0*L1*G1*G2+2.0*L2*G1**2
1161      W(3)=4.0*L1*G1*G3+2.0*L3*G1**2
1162      W(4)=6.0*L2*G2**2
1163      W(5)=4.0*L2*G2*G3+2.0*L3*G2**2
1164      W(6)=4.0*L2*G1*G2+2.0*L1*G2**2
1165      W(7)=6.0*L3*G3**2
1166      W(8)=4.0*L3*G1*G3+2.0*L1*G3**2
1167      W(9)=4.0*L3*G2*G3+2.0*L2*G3**2
1168      W(10)=2.0*(L1*G2*G3+L2*G1*G3+L3*G1*G2)
1169      DO 70 I=1,10
1170          DXX(I)=0.0
1171          DO 60 J=1,10
1172              DXX(I)=DXX(I)+W(J)*GT(TRI,J,I)
1173 60      CONTINUE
1174 70      CONTINUE
1175

```

```

1176      END
1177 *****
1178 * FIND D(PHI)**2/(DX*DU)
1179
1180      SUBROUTINE PHIXU(TRI,L1,L2,L3,F1,F2,F3,G1,G2,G3,DXU)
1181
1182
1183      PARAMETER (MNODE=151 , MNTRIA=50)
1184      DOUBLE PRECISION F1,F2,F3
1185      DOUBLE PRECISION L1,L2,L3,G1,G2,G3,W(10),DXU(10)
1186      DOUBLE PRECISION ML(MNTRIA,10,10)
1187      DOUBLE PRECISION NLM(MNTRIA,16,10,10),NLI(MNTRIA,4,10)
1188      DOUBLE PRECISION MG(MNODE,MNODE)
1189      DOUBLE PRECISION GT(MNTRIA,10,10),LI(MNTRIA,10,4)
1190      INTEGER TRI
1191      COMMON MG,ML,NLM,NLI,LI,GT
1192
1193      W(1)=6.0*L1*F1*G1
1194      W(2)=2.0*L1*(F1*G2+F2*G1)+2.0*L2*F1*G1
1195      W(3)=2.0*L1*(F1*G3+F3*G1)+2.0*L3*F1*G1
1196      W(4)=6.0*L2*F2*G2
1197      W(5)=2.0*L2*(F3*G2+F2*G3)+2.0*L3*F2*G2
1198      W(6)=2.0*L2*(F1*G2+F2*G1)+2.0*L1*F2*G2
1199      W(7)=6.0*L3*F3*G3
1200      W(8)=2.0*L3*(F1*G3+F3*G1)+2.0*L1*F3*G3
1201      W(9)=2.0*L3*(F2*G3+F3*G2)+2.0*L2*F3*G3
1202      W(10)=L1*(F2*G3+F3*G2)+L2*(F1*G3+F3*G1)+L3*(F1*G2+F2*G1)
1203      DO 90 I=1,10
1204          DXU(I)=0.0
1205          DO 80 J=1,10
1206              DXU(I)=DXU(I)+W(J)*GT(TRI,J,I)
1207 80      CONTINUE
1208 90      CONTINUE
1209
1210      END
1211
1212 *****
1213
1214 * DETERMINE ELEMENT CASE, VOLUME, AND DERIV'S OF TETRAHEDRAL
1215 * CO-O RESPECT TO X, U, AND U' COORDINATES
1216
1217      SUBROUTINE CASEDT(TRI,TRIP,CORDND,PTNODE,TIME,E,F,G,U6,
1218 C      CASE,U1,U2,U3,X1,X2,X3)
1219
1220      PARAMETER (MNODE=151 , MNTRIA=50)
1221      DOUBLE PRECISION ML(MNTRIA,10,10)
1222      DOUBLE PRECISION NLM(MNTRIA,16,10,10),NLI(MNTRIA,4,10)
1223      DOUBLE PRECISION MG(MNODE,MNODE)
1224      DOUBLE PRECISION GT(MNTRIA,10,10),LI(MNTRIA,10,4)
1225      DOUBLE PRECISION E(4),F(4),G(4),U6
1226      DOUBLE PRECISION CORDND(MNODE,2),D1,D2
1227      DOUBLE PRECISION U1,U2,U3,B
1228      DOUBLE PRECISION X1,X2,X3,X2P,U1P,U2P,U3P
1229      DOUBLE PRECISION DE(4,4),WK(8),D(4,4)
1230      INTEGER PTNODE(MNTRIA,11),TRI,TRIP,CASE,TIME
1231      COMMON MG,ML,NLM,NLI,LI,GT

```

```

1232
1233     IF (TIME.EQ.1) THEN
1234 * CALCULATE COORDINATES
1235     X1=CORDND(PTNODE(TRI,1),1)
1236     X2=CORDND(PTNODE(TRI,4),1)
1237     X3=CORDND(PTNODE(TRI,7),1)
1238     X1P=CORDND(PTNODE(TRIP,1),1)
1239     U1=CORDND(PTNODE(TRI,1),2)
1240     U2=CORDND(PTNODE(TRI,4),2)
1241     U3=CORDND(PTNODE(TRI,7),2)
1242     U1P=CORDND(PTNODE(TRIP,1),2)
1243     U2P=CORDND(PTNODE(TRIP,4),2)
1244     U3P=CORDND(PTNODE(TRIP,7),2)
1245
1246 * DETERMINE THE CASE OF THE TRIANGLES
1247     CASE=2
1248     IF (X1.NE.X1P) THEN
1249         CASE=1
1250         IF (X1.LT.X1P) THEN
1251             CASE=3
1252         ENDIF
1253     ELSE
1254         IF (X1.GT.X2) THEN
1255             CASE=4
1256         ENDIF
1257     ENDIF
1258 ENDIF
1259
1260 * ASSEMBLE THE COORDINATE TRANSFORMATION MATRIX - DEPENDING
1261 * ON CASE
1262     IF (CASE.EQ.1) THEN
1263         DE(2,1)=X2
1264         DE(2,2)=X1
1265         DE(2,3)=X2
1266         DE(2,4)=X1
1267         DE(3,1)=U2
1268         DE(3,2)=U1
1269         DE(3,3)=U3
1270         DE(3,4)=U1
1271         DE(4,1)=U1P
1272         DE(4,2)=U3P
1273         DE(4,3)=U1P
1274         DE(4,4)=U2P
1275     ENDIF
1276
1277     IF (CASE.EQ.3) THEN
1278         DE(2,1)=X2
1279         DE(2,2)=X2
1280         DE(2,3)=X1
1281         DE(2,4)=X1
1282         DE(3,1)=U2
1283         DE(3,2)=U3
1284         DE(3,3)=U1
1285         DE(3,4)=U1
1286         DE(4,1)=U1P
1287         DE(4,2)=U1P

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```

1288         DE(4,3)=U3P
1289         DE(4,4)=U2P
1290     ENDIF
1291
1292     IF (CASE.EQ.2) THEN
1293         DE(2,1)=X1
1294         DE(2,2)=X2
1295         DE(2,3)=X2
1296         DE(2,4)=X2
1297         DE(3,1)=U1
1298         DE(3,2)=U3
1299         DE(3,3)=U2
1300         DE(3,4)=U3
1301         DE(4,1)=U1P
1302         DE(4,2)=U3P
1303         DE(4,3)=U2P
1304         DE(4,4)=U2P
1305         IF (TIME.EQ.2) THEN
1306             DE(3,2)=U2
1307             DE(3,3)=U3
1308             DE(3,4)=U2
1309             DE(4,2)=U2P
1310             DE(4,3)=U3P
1311             DE(4,4)=U3P
1312         ENDIF
1313     ENDIF
1314
1315     IF (CASE.EQ.4) THEN
1316         DE(2,1)=X1
1317         DE(2,2)=X2
1318         DE(2,3)=X2
1319         DE(2,4)=X2
1320         DE(3,1)=U1
1321         DE(3,2)=U3
1322         DE(3,3)=U2
1323         DE(3,4)=U2
1324         DE(4,1)=U1P
1325         DE(4,2)=U3P
1326         DE(4,3)=U2P
1327         DE(4,4)=U3P
1328         IF (TIME.EQ.2) THEN
1329             DE(3,2)=U2
1330             DE(3,3)=U3
1331             DE(3,4)=U3
1332             DE(4,2)=U2P
1333             DE(4,3)=U3P
1334             DE(4,4)=U2P
1335         ENDIF
1336     ENDIF
1337
1338     DO 10 I=1,4
1339         DE(1,I)=1.0
1340 10 CONTINUE
1341
1342 * COPY MATRIX TO AVOID DECOMPOSITION BY IMSL
1343     DO 17 I=1,4

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```

1344          DO 15 J=1,4
1345             D(I,J)=DE(I,J)
1346 15        CONTINUE
1347 17        CONTINUE
1348
1349 * FIND VOLUME FROM MATRIX DETERMINATE
1350          D1=0.0
1351          CALL LINV3F(DE,B,4,4,4,D1,D2,WK,IER)
1352          V6=D1*2**D2
1353
1354 * DERIVATIVES OF NATURAL COORDINATES
1355          D1=-1.0
1356          CALL LINV3F(D,B,1,4,4,D1,D2,WK,IER)
1357          DO 20 I=1,4
1358             E(I)=D(I,2)
1359             F(I)=D(I,3)
1360             G(I)=D(I,4)
1361 20        CONTINUE
1362
1363          END
1364
1365 *****
1366          SUBROUTINE SINFCN(E,F,G,V,SGM,H)
1367
1368          PARAMETER (MNODE=151 , MNTRIA=50)
1369
1370 * FIND THE INTERPOLATING FUNCTION MATRIX (20 X 20 FOR A CUBIC
1371 * IN 3THEN MULTIPLY BY THE Vi's TO GET THE Mi's
1372 * (THESIS NOTATION)
1373 * RESULT ARE THE BASIS FUNCTIONS FOR THE TETRAHEDRAL CUBIC
1374
1375          DOUBLE PRECISION ML(MNTRIA,10,10)
1376          DOUBLE PRECISION NLM(MNTRIA,16,10,10),NLI(MNTRIA,4,10)
1377          DOUBLE PRECISION MG(MNODE,MNODE)
1378          DOUBLE PRECISION GT(MNTRIA,10,10),LI(MNTRIA,10,4)
1379          DOUBLE PRECISION M(17,4,4),SGT(20,20),WK(8),W(4,4)
1380          DOUBLE PRECISION SGM(5,4,4),E(4),F(4),G(4),V(5,20)
1381          DOUBLE PRECISION H(5,20),A,B,C,D1,D2,MT(4,4)
1382          COMMON MG,ML,NLM,NLI,LI,GT
1383
1384
1385 * ZERO THE TETRAHEDRAL INTERPOLATING FUNCTION MATRIX
1386          DO 10 I=1,20
1387             DO 5 J=1,20
1388                SGT(I,J)=0.0
1389 5          CONTINUE
1390 10        CONTINUE
1391
1392 * ASSEMBLE THE PARTITIONED MATRICES ON THE DIAGONAL
1393          DO 30 K=1,4
1394             DO 20 J=1,4
1395                M(K,1,J)=1.0*(1/J)
1396                M(K,2,J)=3.0*E(J)-((J+1)/3)*2.0*E(J)
1397                M(K,3,J)=3.0*F(J)-((J+1)/3)*2.0*F(J)
1398                M(K,4,J)=3.0*G(J)-((J+1)/3)*2.0*G(J)
1399 20        CONTINUE

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```

2128      F(14,5,8)=1.0
2129      F(16,5,9)=1.0
2130      L1=0.0
2131      L2=1.0
2132      L3=0.0
2133      CALL PHIXX(TRI,L1,L2,L3,G1,G2,G3,W1)
2134      CALL PHIXU(TRI,L1,L2,L3,F1,F2,F3,G1,G2,G3,W2)
2135      L1=1.0
2136      L2=0.0
2137      CALL PHIXX(TRI,L1,L2,L3,G1,G2,G3,W3)
2138      CALL PHIXU(TRI,L1,L2,L3,F1,F2,F3,G1,G2,G3,W4)
2139      L1=0.0
2140      L3=1.0
2141      CALL PHIXX(TRI,L1,L2,L3,G1,G2,G3,W5)
2142      CALL PHIXU(TRI,L1,L2,L3,F1,F2,F3,G1,G2,G3,W6)
2143      DO 150 I=1,10
2144          F(2,I,1)=W3(I)
2145          F(3,I,1)=W4(I)
2146          F(6,I,7)=W5(I)
2147          F(7,I,7)=W6(I)
2148          F(10,I,4)=W1(I)
2149          F(11,I,4)=W2(I)
2150          F(14,I,7)=W1(I)
2151          F(15,I,7)=W2(I)
2152 150      CONTINUE
2153      L1=0.0
2154      L2=2.0/3.0
2155      L3=1.0/3.0
2156      CALL PHIX(TRI,L1,L2,L3,G1,G2,G3,W1)
2157      L2=1.0/3.0
2158      L3=2.0/3.0
2159      CALL PHII(TRIP,L1,L2,L3,W2)
2160      L1=1.0/3.0
2161      L2=2.0/3.0
2162      L3=0.0
2163      CALL PHIX(TRI,L1,L2,L3,G1,G2,G3,W3)
2164      L2=0.0
2165      L3=2.0/3.0
2166      CALL PHII(TRIP,L1,L2,L3,W4)
2167      L3=1.0/3.0
2168      L2=1.0/3.0
2169      CALL PHIX(TRI,L1,L2,L3,G1,G2,G3,W5)
2170      DO 170 I=1,10
2171          F(18,I,10)=W3(I)
2172          F(20,I,10)=W5(I)
2173          DO 160 J=1,10
2174              F(17,I,J)=W1(I)*W2(J)
2175              F(19,I,J)=W5(I)*W4(J)
2176 160      CONTINUE
2177 170      CONTINUE
2178      ELSE
2179          IF (CASE.EQ.4.AND.TIME.EQ.2) THEN
2180              UU(1)=U1
2181              UU(2)=U2
2182              UU(3)=U3
2183              UU(4)=U3

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```

2072      L3=1.0
2073      CALL PHIXX(TRI,L1,L2,L3,G1,G2,G3,W5)
2074      CALL PHIXU(TRI,L1,L2,L3,F1,F2,F3,G1,G2,G3,W6)
2075          DO 120 I=1,10
2076              F(2,I,1)=W3(I)
2077              F(3,I,1)=W4(I)
2078              F(6,I,4)=W1(I)
2079              F(7,I,4)=W2(I)
2080              F(10,I,7)=W5(I)
2081              F(11,I,7)=W6(I)
2082              F(14,I,7)=W1(I)
2083              F(15,I,7)=W2(I)
2084 120      CONTINUE
2085          L1=0.0
2086          L2=2.0/3.0
2087          L3=1.0/3.0
2088          CALL PHIX(TRI,L1,L2,L3,G1,G2,G3,W1)
2089          L2=1.0/3.0
2090          L3=2.0/3.0
2091          CALL PHII(TRIP,L1,L2,L3,W2)
2092          L1=1.0/3.0
2093          L2=0.0
2094          L3=2.0/3.0
2095          CALL PHII(TRIP,L1,L2,L3,W3)
2096          L2=2.0/3.0
2097          L3=0.0
2098          CALL PHIX(TRI,L1,L2,L3,G1,G2,G3,W4)
2099          L2=1.0/3.0
2100          L3=1.0/3.0
2101          CALL PHIX(TRI,L1,L2,L3,G1,G2,G3,W5)
2102          DO 140 I=1,10
2103              DO 130 J=1,10
2104                  F(17,I,J)=W1(I)*W2(J)
2105                  F(18,I,J)=W5(I)*W3(J)
2106 130      CONTINUE
2107          F(19,I,10)=W4(I)
2108          F(20,I,10)=W5(I)
2109 140      CONTINUE
2110      ENDIF
2111  ENDIF
2112
2113  IF (CASE.EQ.4.AND.TIME.EQ.1) THEN
2114      UU(1)=U1
2115      UU(2)=U3
2116      UU(3)=U2
2117      UU(4)=U2
2118      F(1,2,1)=1.0
2119      F(2,2,2)=1.0
2120      F(4,2,3)=1.0
2121      F(5,8,7)=1.0
2122      F(6,8,8)=1.0
2123      F(8,8,9)=1.0
2124      F(9,5,4)=1.0
2125      F(10,5,5)=1.0
2126      F(12,5,6)=1.0
2127      F(13,5,7)=1.0

```

```

2016          F(14,I,4)=W5(I)
2017          F(15,I,4)=W6(I)
2018 90        CONTINUE
2019          L1=0.0
2020          L2=1.0/3.0
2021          L3=2.0/3.0
2022          CALL PHIX(TRI,L1,L2,L3,G1,G2,G3,W1)
2023          L2=2.0/3.0
2024          L3=1.0/3.0
2025          CALL PHII(TRIP,L1,L2,L3,W2)
2026          L1=1.0/3.0
2027          L2=2.0/3.0
2028          L3=0.0
2029          CALL PHII(TRIP,L1,L2,L3,W3)
2030          L2=0.0
2031          L3=2.0/3.0
2032          CALL PHIX(TRI,L1,L2,L3,G1,G2,G3,W4)
2033          L3=1.0/3.0
2034          L2=1.0/3.0
2035          CALL PHIX(TRI,L1,L2,L3,G1,G2,G3,W5)
2036          DO 110 I=1,10
2037              F(19,I,10)=W4(I)
2038              F(20,I,10)=W5(I)
2039              DO 100 J=1,10
2040                  F(17,I,J)=W1(I)*W2(J)
2041                  F(18,I,J)=W5(I)*W3(J)
2042 100        CONTINUE
2043 110        CONTINUE
2044      ELSE
2045          IF (CASE.EQ.2.AND.TIME.EQ.2) THEN
2046              UU(1)=U1
2047              UU(2)=U2
2048              UU(3)=U3
2049              UU(4)=U2
2050              F(1,2,1)=1.0
2051              F(2,2,2)=1.0
2052              F(4,2,3)=1.0
2053              F(5,5,4)=1.0
2054              F(6,5,5)=1.0
2055              F(8,5,6)=1.0
2056              F(9,8,7)=1.0
2057              F(10,8,8)=1.0
2058              F(12,8,9)=1.0
2059              F(13,5,7)=1.0
2060              F(14,5,8)=1.0
2061              F(16,5,9)=1.0
2062              L1=0.0
2063              L2=1.0
2064              L3=0.0
2065              CALL PHIXX(TRI,L1,L2,L3,G1,G2,G3,W1)
2066              CALL PHIXU(TRI,L1,L2,L3,F1,F2,F3,G1,G2,G3,W2)
2067              L1=1.0
2068              L2=0.0
2069              CALL PHIXX(TRI,L1,L2,L3,G1,G2,G3,W3)
2070              CALL PHIXU(TRI,L1,L2,L3,F1,F2,F3,G1,G2,G3,W4)
2071          L1=0.0

```

```

1960      CALL PHIX(TRI,L1,L2,L3,G1,G2,G3,W1)
1961      CALL PHII(TRIP,L1,L2,L3,W6)
1962      L2=1.0/3.0
1963      L3=0.0
1964      CALL PHIX(TRI,L1,L2,L3,G1,G2,G3,W2)
1965      CALL PHII(TRIP,L1,L2,L3,W5)
1966      L1=L2
1967      L3=L1
1968      CALL PHIX(TRI,L1,L2,L3,G1,G2,G3,W3)
1969      DO 80 I=1,10
1970          F(17,I,10)=W1(I)
1971          F(18,I,10)=W2(I)
1972          DO 70 J=1,10
1973              F(19,I,J)=W3(I)*W5(J)
1974              F(20,I,J)=W3(I)*W6(J)
1975 70      CONTINUE
1976 80      CONTINUE
1977      ENDIF
1978
1979      IF (CASE.EQ.2.AND.TIME.EQ.1) THEN
1980          UU(1)=U1
1981          UU(2)=U3
1982          UU(3)=U2
1983          UU(4)=U3
1984          F(1,2,1)=1.0
1985          F(2,2,2)=1.0
1986          F(4,2,3)=1.0
1987          F(5,8,7)=1.0
1988          F(6,8,8)=1.0
1989          F(8,8,9)=1.0
1990          F(9,5,4)=1.0
1991          F(10,5,5)=1.0
1992          F(12,5,6)=1.0
1993          F(13,8,4)=1.0
1994          F(14,8,5)=1.0
1995          F(16,8,6)=1.0
1996          L1=0.0
1997          L2=1.0
1998          L3=0.0
1999          CALL PHIXX(TRI,L1,L2,L3,G1,G2,G3,W1)
2000          CALL PHIXU(TRI,L1,L2,L3,F1,F2,F3,G1,G2,G3,W2)
2001          L1=1.0
2002          L2=0.0
2003          CALL PHIXX(TRI,L1,L2,L3,G1,G2,G3,W3)
2004          CALL PHIXU(TRI,L1,L2,L3,F1,F2,F3,G1,G2,G3,W4)
2005          L1=0.0
2006          L3=1.0
2007          CALL PHIXX(TRI,L1,L2,L3,G1,G2,G3,W5)
2008          CALL PHIXU(TRI,L1,L2,L3,F1,F2,F3,G1,G2,G3,W6)
2009          DO 90 I=1,10
2010              F(2,I,1)=W3(I)
2011              F(3,I,1)=W4(I)
2012              F(6,I,7)=W5(I)
2013              F(7,I,7)=W6(I)
2014              F(10,I,4)=W1(I)
2015              F(11,I,4)=W2(I)

```

```

1904      L3=0.0
1905      CALL PHII(TRIP,L1,L2,L3,W2)
1906      L2=0.0
1907      L3=1.0/3.0
1908      CALL PHII(TRIP,L1,L2,L3,W3)
1909      DO 40 I=1,10
1910          DO 30 J=1,10
1911              F(18,I,J)=W1(I)*W2(J)
1912              F(20,I,J)=W1(I)*W3(J)
1913 30      CONTINUE
1914 40      CONTINUE
1915      ENDIF
1916
1917      IF (CASE.EQ.3) THEN
1918          UU(1)=U2
1919          UU(2)=U3
1920          UU(3)=U1
1921          UU(4)=U1
1922          F(1,5,1)=1.0
1923          F(2,5,2)=1.0
1924          F(4,5,3)=1.0
1925          F(5,8,1)=1.0
1926          F(6,8,2)=1.0
1927          F(8,8,3)=1.0
1928          F(9,2,7)=1.0
1929          F(10,2,8)=1.0
1930          F(12,2,9)=1.0
1931          F(13,2,4)=1.0
1932          F(14,2,5)=1.0
1933          F(16,2,6)=1.0
1934          L1=0.0
1935          L2=1.0
1936          L3=0.0
1937          CALL PHIXX(TRI,L1,L2,L3,G1,G2,G3,W1)
1938          CALL PHIXU(TRI,L1,L2,L3,F1,F2,F3,G1,G2,G3,W2)
1939          L1=1.0
1940          L2=0.0
1941          CALL PHIXX(TRI,L1,L2,L3,G1,G2,G3,W3)
1942          CALL PHIXU(TRI,L1,L2,L3,F1,F2,F3,G1,G2,G3,W4)
1943          L1=0.0
1944          L3=1.0
1945          CALL PHIXX(TRI,L1,L2,L3,G1,G2,G3,W5)
1946          CALL PHIXU(TRI,L1,L2,L3,F1,F2,F3,G1,G2,G3,W6)
1947          DO 60 I=1,10
1948              F(2,I,1)=W1(I)
1949              F(3,I,1)=W2(I)
1950              F(6,I,1)=W5(I)
1951              F(7,I,1)=W6(I)
1952              F(10,I,7)=W3(I)
1953              F(11,I,7)=W4(I)
1954              F(14,I,4)=W3(I)
1955              F(15,I,4)=W4(I)
1956 60      CONTINUE
1957          L1=2.0/3.0
1958          L2=0.0
1959          L3=1.0/3.0

```

```

1848 * F1'S BY CASE
1849     IF (CASE.EQ.1) THEN
1850         UU(1)=U2
1851         UU(2)=U1
1852         UU(3)=U3
1853         UU(4)=U1
1854         F(1,5,1)=1.0
1855         F(2,5,2)=1.0
1856         F(4,5,3)=1.0
1857         F(5,2,7)=1.0
1858         F(6,2,8)=1.0
1859         F(8,2,9)=1.0
1860         F(9,8,1)=1.0
1861         F(10,8,2)=1.0
1862         F(12,8,3)=1.0
1863         F(13,2,4)=1.0
1864         F(14,2,5)=1.0
1865         F(16,2,6)=1.0
1866         L1=0.0
1867         L2=1.0
1868         L3=0.0
1869         CALL PHIXX(TRI,L1,L2,L3,G1,G2,G3,W1)
1870         CALL PHIXU(TRI,L1,L2,L3,F1,F2,F3,G1,G2,G3,W2)
1871         L1=1.0
1872         L2=0.0
1873         CALL PHIXX(TRI,L1,L2,L3,G1,G2,G3,W3)
1874         CALL PHIXU(TRI,L1,L2,L3,F1,F2,F3,G1,G2,G3,W4)
1875         L1=0.0
1876         L3=1.0
1877         CALL PHIXX(TRI,L1,L2,L3,G1,G2,G3,W5)
1878         CALL PHIXU(TRI,L1,L2,L3,F1,F2,F3,G1,G2,G3,W6)
1879         DO 10 I=1,10
1880             F(2,I,1)=W1(I)
1881             F(3,I,1)=W2(I)
1882             F(6,I,7)=W3(I)
1883             F(7,I,7)=W4(I)
1884             F(10,I,1)=W5(I)
1885             F(11,I,1)=W6(I)
1886             F(14,I,4)=W3(I)
1887             F(15,I,4)=W4(I)
1888 10     CONTINUE
1889         L1=2.0/3.0
1890         L2=0.0
1891         L3=1.0/3.0
1892         CALL PHIX(TRI,L1,L2,L3,G1,G2,G3,W1)
1893         L2=1.0/3.0
1894         L3=0.0
1895         CALL PHIX(TRI,L1,L2,L3,G1,G2,G3,W2)
1896         DO 20 I=1,10
1897             F(17,I,10)=W1(I)
1898             F(19,I,10)=W2(I)
1899 20     CONTINUE
1900         L1=1.0/3.0
1901         L3=1.0/3.0
1902         CALL PHIX(TRI,L1,L2,L3,G1,G2,G3,W1)
1903         L1=2.0/3.0

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1792 * MULTIPLY BY HI'S AND SUM TO FIND THE SCATTERING CONTRIBUTION
1793 * FROM THE (PHI)*(PHI') TERM
1794     DO 260 K=1,20
1795         DO 250 I=1,10
1796             DO 240 J=1,10
1797                 SA(I,J)=SA(I,J)+H(1,K)*F(K,I,J)
1798 240         CONTINUE
1799 250     CONTINUE
1800 260     CONTINUE
1801
1802
1803     END
1804 *****
1805
1806 * SECOND SCATTERING INTEGRAL ( D(PHI)/DX * PHI' )
1807
1808     SUBROUTINE SCATB(U1,U2,U3,X1,X2,X3,TRI,TRIP,AREAS,H
1809 C         ,CASE,TIME,SB,CORDND,PTNODE)
1810
1811
1812     PARAMETER (MNODE=151 , MNTRIA=50)
1813
1814     DOUBLE PRECISION U1,U2,U3,X1,X2,X3,AREAS(MNTRIA)
1815     DOUBLE PRECISION SB(10,10),W6(10)
1816     DOUBLE PRECISION A,G1,G2,G3,F1,F2,F3
1817     DOUBLE PRECISION CORDND(MNODE,2)
1818     DOUBLE PRECISION W1(10),W2(10),W3(10),W4(10),W5(10)
1819     DOUBLE PRECISION F(20,10,10),L1,L2,L3,H(5,20),UU(4)
1820     DOUBLE PRECISION ML(MNTRIA,10,10)
1821     DOUBLE PRECISION NLN(MNTRIA,16,10,10),NLI(MNTRIA,4,10)
1822     DOUBLE PRECISION MG(MNODE,MNODE)
1823     DOUBLE PRECISION GT(MNTRIA,10,10),LI(MNTRIA,10,4)
1824     INTEGER CASE,TIME,TRI,TRIP
1825     INTEGER PTNODE(MNTRIA,11)
1826     COMMON MG,ML,NLN,NLI,LI,GT
1827
1828 * ZERO THE F MATRICES
1829     DO 7 K=1,20
1830         DO 6 I=1,10
1831             DO 5 J=1,10
1832                 F(K,I,J)=0.0
1833 5         CONTINUE
1834 6     CONTINUE
1835 7     CONTINUE
1836
1837 * DERIVATIVES OF TRIANGULAR COORDINATES W.R.T. SPATIAL
1838 * VARIABLES
1839     A=2.0*AREAS(TRI)
1840     G1=(U2-U3)/A
1841     G2=(U3-U1)/A
1842     G3=(U1-U2)/A
1843     F1=(X3-X2)/A
1844     F2=(X1-X3)/A
1845     F3=(X2-X1)/A
1846
1847 * ASSIGN THE U COORDS OF TETRAHEDRAL NODES AND ASSEMBLE THE

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```

1736      ELSE
1737          IF (CASE.EQ.4.AND.TIME.EQ.2) THEN
1738              F(1,1,1)=1.0
1739              F(2,1,2)=1.0
1740              F(2,2,1)=1.0
1741              F(3,3,1)=1.0
1742              F(4,1,3)=1.0
1743              F(5,4,4)=1.0
1744              F(6,5,4)=1.0
1745              F(6,4,5)=1.0
1746              F(7,6,4)=1.0
1747              F(8,4,6)=1.0
1748              F(9,7,7)=1.0
1749              F(10,8,7)=1.0
1750              F(10,7,8)=1.0
1751              F(11,9,7)=1.0
1752              F(12,7,9)=1.0
1753              F(13,7,4)=1.0
1754              F(14,8,4)=1.0
1755              F(14,7,5)=1.0
1756              F(15,9,4)=1.0
1757              F(16,7,6)=1.0
1758              F(20,10,10)=1.0
1759              L1=0.0
1760              L2=1.0/3.0
1761              L3=2.0/3.0
1762              CALL PHII(TRI,L1,L2,L3,W1)
1763              L2=2.0/3.0
1764              L3=1.0/3.0
1765              CALL PHII(TRIP,L1,L2,L3,W2)
1766              DO 190 I=1,10
1767                  DO 180 J=1,10
1768                      F(17,I,J)=W1(I)*W2(J)
1769 180              CONTINUE
1770 190              CONTINUE
1771              L1=1.0/3.0
1772              L2=0.0
1773              L3=2.0/3.0
1774              CALL PHII(TRI,L1,L2,L3,W2)
1775              L2=2.0/3.0
1776              L3=0.0
1777              CALL PHII(TRIP,L1,L2,L3,W1)
1778              DO 200 I=1,10
1779                  F(18,I,10)=W2(I)
1780                  F(19,10,I)=W1(I)
1781 200              CONTINUE
1782              ENDIF
1783          ENDIF
1784
1785      * ZERO THE SCATTERING MATRIX
1786      DO 230 I=1,10
1787          DO 220 J=1,10
1788              SA(I,J)=0.0
1789 220          CONTINUE
1790 230          CONTINUE
1791

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```

1680          CALL PHII(TRIP,L1,L2,L3,W2)
1681          L2=2.0/3.0
1682          L3=0.0
1683          CALL PHII(TRI,L1,L2,L3,W1)
1684          DO 120 I=1,10
1685              F(18,10,I)=W2(I)
1686              F(19,I,10)=W1(I)
1687 120          CONTINUE
1688          ENDIF
1689      ENDIF
1690
1691      IF (CASE.EQ.4.AND.TIME.EQ.1) THEN
1692          F(1,1,1)=1.0
1693          F(2,1,2)=1.0
1694          F(2,2,1)=1.0
1695          F(3,3,1)=1.0
1696          F(4,1,3)=1.0
1697          F(5,7,7)=1.0
1698          F(6,7,8)=1.0
1699          F(6,8,7)=1.0
1700          F(7,9,7)=1.0
1701          F(8,7,9)=1.0
1702          F(9,4,4)=1.0
1703          F(10,4,5)=1.0
1704          F(10,5,4)=1.0
1705          F(11,6,4)=1.0
1706          F(12,4,6)=1.0
1707          F(20,10,10)=1.0
1708          F(13,4,7)=1.0
1709          F(14,5,7)=1.0
1710          F(14,4,8)=1.0
1711          F(15,6,7)=1.0
1712          F(16,4,9)=1.0
1713          L1=0.0
1714          L2=2.0/3.0
1715          L3=1.0/3.0
1716          CALL PHII(TRI,L1,L2,L3,W1)
1717          L2=1.0/3.0
1718          L3=2.0/3.0
1719          CALL PHII(TRIP,L1,L2,L3,W2)
1720          DO 160 I=1,10
1721              DO 150 J=1,10
1722                  F(17,I,J)=W1(I)*W2(J)
1723 150          CONTINUE
1724 160          CONTINUE
1725          L1=1.0/3.0
1726          L2=2.0/3.0
1727          L3=0.0
1728          CALL PHII(TRI,L1,L2,L3,W2)
1729          L2=0.0
1730          L3=2.0/3.0
1731          CALL PHII(TRIP,L1,L2,L3,W1)
1732          DO 170 I=1,10
1733              F(18,I,10)=W2(I)
1734              F(19,10,I)=W1(I)
1735 170          CONTINUE

```

```

1624      L3=1.0/3.0
1625      CALL PHII(TRIP,L1,L2,L3,W2)
1626      DO 80 I=1,10
1627          DO 70 J=1,10
1628              F(17,I,J)=W1(I)*W2(J)
1629 70      CONTINUE
1630 80      CONTINUE
1631      L1=1.0/3.0
1632      L2=2.0/3.0
1633      L3=0.0
1634      CALL PHII(TRIP,L1,L2,L3,W2)
1635      L2=0.0
1636      L3=2.0/3.0
1637      CALL PHII(TRI,L1,L2,L3,W1)
1638      DO 90 I=1,10
1639          F(18,10,I)=W2(I)
1640          F(19,I,10)=W1(I)
1641 90      CONTINUE
1642  ELSE
1643      IF (CASE.EQ.2.AND.TIME.EQ.2) THEN
1644          F(1,1,1)=1.0
1645          F(2,1,2)=1.0
1646          F(2,2,1)=1.0
1647          F(3,3,1)=1.0
1648          F(4,1,3)=1.0
1649          F(5,4,4)=1.0
1650          F(6,5,4)=1.0
1651          F(6,4,5)=1.0
1652          F(7,6,4)=1.0
1653          F(8,4,6)=1.0
1654          F(9,7,7)=1.0
1655          F(10,8,7)=1.0
1656          F(10,7,8)=1.0
1657          F(11,9,7)=1.0
1658          F(12,7,9)=1.0
1659          F(13,4,7)=1.0
1660          F(14,4,8)=1.0
1661          F(14,5,7)=1.0
1662          F(15,6,7)=1.0
1663          F(16,4,9)=1.0
1664          F(20,10,10)=1.0
1665          L1=0.0
1666          L2=2.0/3.0
1667          L3=1.0/3.0
1668          CALL PHII(TRI,L1,L2,L3,W1)
1669          L2=1.0/3.0
1670          L3=2.0/3.0
1671          CALL PHII(TRIP,L1,L2,L3,W2)
1672          DO 110 I=1,10
1673              DO 100 J=1,10
1674                  F(17,I,J)=W1(I)*W2(J)
1675 100      CONTINUE
1676 110      CONTINUE
1677          L1=1.0/3.0
1678          L2=0.0
1679          L3=2.0/3.0

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```

1568      F(9,1,7)=1.0
1569      F(10,1,8)=1.0
1570      F(10,2,7)=1.0
1571      F(11,3,7)=1.0
1572      F(12,1,9)=1.0
1573      F(13,1,4)=1.0
1574      F(14,1,5)=1.0
1575      F(14,2,4)=1.0
1576      F(15,3,4)=1.0
1577      F(16,1,6)=1.0
1578      L1=2.0/3.0
1579      L2=0.0
1580      L3=1.0/3.0
1581      CALL PHII(TRI,L1,L2,L3,W1)
1582      CALL PHII(TRIP,L1,L2,L3,W2)
1583      DO 50 I=1,10
1584          F(17,I,10)=W1(I)
1585          F(20,10,I)=W2(I)
1586 50      CONTINUE
1587      L2=1.0/3.0
1588      L3=0.0
1589      CALL PHII(TRI,L1,L2,L3,W1)
1590      CALL PHII(TRIP,L1,L2,L3,W2)
1591      DO 60 I=1,10
1592          F(18,I,10)=W1(I)
1593          F(19,10,I)=W2(I)
1594 60      CONTINUE
1595      ENDIF
1596
1597      IF (CASE.EQ.2.AND.TIME.EQ.1) THEN
1598          F(1,1,1)=1.0
1599          F(2,1,2)=1.0
1600          F(2,2,1)=1.0
1601          F(3,3,1)=1.0
1602          F(4,1,3)=1.0
1603          F(5,7,7)=1.0
1604          F(6,7,8)=1.0
1605          F(6,8,7)=1.0
1606          F(7,9,7)=1.0
1607          F(8,7,9)=1.0
1608          F(9,4,4)=1.0
1609          F(10,4,5)=1.0
1610          F(10,5,4)=1.0
1611          F(11,6,4)=1.0
1612          F(12,4,6)=1.0
1613          F(13,7,4)=1.0
1614          F(14,7,5)=1.0
1615          F(14,8,4)=1.0
1616          F(15,9,4)=1.0
1617          F(16,7,6)=1.0
1618          F(20,10,10)=1.0
1619          L1=0.0
1620          L2=1.0/3.0
1621          L3=2.0/3.0
1622          CALL PHII(TRI,L1,L2,L3,W1)
1623          L2=2.0/3.0

```

```

1512 20          CONTINUE
1513 30          CONTINUE
1514
1515 * INITIALIZE THE Fi'S DEPENDING UPON THE TETRAHEDRAL CASE
1516 * AND TIME
1517     IF (CASE.EQ.1) THEN
1518         F(1,4,1)=1.0
1519         F(2,4,2)=1.0
1520         F(2,5,1)=1.0
1521         F(3,6,1)=1.0
1522         F(4,4,3)=1.0
1523         F(5,1,7)=1.0
1524         F(6,1,8)=1.0
1525         F(6,2,7)=1.0
1526         F(7,3,7)=1.0
1527         F(8,1,9)=1.0
1528         F(9,7,1)=1.0
1529         F(10,8,1)=1.0
1530         F(10,7,2)=1.0
1531         F(11,9,1)=1.0
1532         F(12,7,3)=1.0
1533         F(13,1,4)=1.0
1534         F(14,1,5)=1.0
1535         F(14,2,4)=1.0
1536         F(15,3,4)=1.0
1537         F(16,1,6)=1.0
1538         L1=2.0/3.0
1539         L2=0.0
1540         L3=1.0/3.0
1541         CALL PHII(TRI,L1,L2,L3,W1)
1542         CALL PHII(TRIP,L1,L2,L3,W2)
1543         DO 32 I=1,10
1544             F(17,I,10)=W1(I)
1545             F(20,10,I)=W2(I)
1546 32      CONTINUE
1547         L2=1.0/3.0
1548         L3=0.0
1549         CALL PHII(TRI,L1,L2,L3,W1)
1550         CALL PHII(TRIP,L1,L2,L3,W2)
1551         DO 34 I=1,10
1552             F(18,10,I)=W2(I)
1553             F(19,I,10)=W1(I)
1554 34      CONTINUE
1555     ENDIF
1556
1557     IF (CASE.EQ.3) THEN
1558         F(1,4,1)=1.0
1559         F(2,4,2)=1.0
1560         F(2,5,1)=1.0
1561         F(3,6,1)=1.0
1562         F(4,4,3)=1.0
1563         F(5,7,1)=1.0
1564         F(6,8,1)=1.0
1565         F(6,7,2)=1.0
1566         F(7,9,1)=1.0
1567         F(8,7,3)=1.0

```

```

1456             SGT(I+12,J+12)=M(12,I,J)
1457 160         CONTINUE
1458 170         CONTINUE
1459             DO 190 I=17,20
1460                 DO 180 J=1,16
1461                     K=((J-1)/4)+13
1462                     L=J-(K-13)*4
1463                     SGT(I,J)=M(K,I-16,L)
1464 180         CONTINUE
1465 190         CONTINUE
1466
1467             DO 197 I=17,20
1468                 DO 195 J=17,20
1469                     SGT(I,J)=SGM(5,I-16,J-16)
1470 195         CONTINUE
1471 197         CONTINUE
1472
1473 * FIND THE Hi'S
1474             DO 220 I=1,5
1475                 DO 210 J=1,20
1476                     H(I,J)=0.0
1477                     DO 200 L=1,20
1478                         H(I,J)=H(I,J)+V(I,L)*SGT(L,J)
1479 200         CONTINUE
1480 210         CONTINUE
1481 220         CONTINUE
1482
1483         END
1484 *****
1485
1486 * CALCULATE THE FIRST ( PHI*PHI' ) SCATTERING INTEGRAL
1487 * CUBIC FIT OVER A TETRAHEDRON WITH CORNER FLUXES, GRADIENTS
1488 * AND FACE CENTERED FLUXES AS DEGREES OF FREEDOM
1489
1490         SUBROUTINE SCATA(H,TRI,TRIP,CASE,TIME,SA,CORDND,PTNODE)
1491
1492         PARAMETER (MNODE=151 , MNTRIA=50)
1493
1494         DOUBLE PRECISION ML(MNTRIA,10,10)
1495         DOUBLE PRECISION NLM(MNTRIA,16,10,10),NLI(MNTRIA,4,10)
1496         DOUBLE PRECISION MG(MNODE,MNODE)
1497         DOUBLE PRECISION GT(MNTRIA,10,10),LI(MNTRIA,10,4)
1498         DOUBLE PRECISION X2,X2P,U2,U2P,CORDND(MNODE,2)
1499         DOUBLE PRECISION F(20,10,10),W1(10),W2(10),L1,L2,L3
1500         DOUBLE PRECISION SA(10,10)
1501         DOUBLE PRECISION H(5,20)
1502         INTEGER TRI,TRIP,CASE,TIME
1503         INTEGER PTNODE(MNTRIA,11)
1504         COMMON MG,ML,NLM,NLI,LI,GT
1505
1506 * ZERO THE Fi'S
1507             DO 30 I=1,20
1508                 DO 20 J=1,10
1509                     DO 10 K=1,10
1510                         F(I,J,K)=0.0
1511 10         CONTINUE

```

```

1400      A=E(1)
1401      B=F(1)
1402      C=G(1)
1403      IF (K.LT.4) THEN
1404          E(1)=E(K+1)
1405          F(1)=F(K+1)
1406          G(1)=G(K+1)
1407          E(K+1)=A
1408          F(K+1)=B
1409          G(K+1)=C
1410      ENDIF
1411 30      CONTINUE
1412
1413 * TAKE INVERSES OF MATRICES 1-4
1414      DO 80 K=1,4
1415          DO 50 I=1,4
1416              DO 40 J=1,4
1417                  W(I,J)=M(K,I,J)
1418          40      CONTINUE
1419      50      CONTINUE
1420      D1=-1.0
1421      CALL LINV3F(W,B,1,4,4,D1,D2,WK,IER)
1422      DO 70 I=1,4
1423          DO 60 J=1,4
1424              M(K+8,I,J)=W(I,J)
1425      60      CONTINUE
1426      70      CONTINUE
1427      80      CONTINUE
1428
1429 * FIND REMAINING SUB MATRICES
1430      DO 150 K=13,16
1431          DO 110 I=1,4
1432              DO 100 J=1,4
1433                  MT(I,J)=0.0
1434                  DO 90 L=1,4
1435                      MT(I,J)=MT(I,J)+SGM(K-12,I,L)*M(K-4,L,J)
1436      90      CONTINUE
1437      100      CONTINUE
1438      110      CONTINUE
1439      DO 140 I=1,4
1440          DO 130 J=1,4
1441              M(K,I,J)=0.0
1442              DO 120 L=1,4
1443                  M(K,I,J)=M(K,I,J)-SGM(5,I,L)*MT(L,J)
1444      120      CONTINUE
1445      130      CONTINUE
1446      140      CONTINUE
1447      150      CONTINUE
1448
1449 * ASSEMBLE INTO THE TETRAHEDRAL (SCATTERING) INTERPOLATING
1450 * FUNCTION MATRIX OF CONSTANTS
1451      DO 170 I=1,4
1452          DO 160 J=1,4
1453              SGT(I,J)=M(9,I,J)
1454              SGT(I+4,J+4)=M(10,I,J)
1455              SGT(I+8,J+8)=M(11,I,J)

```

```

2184      F(1,2,1)=1.0
2185      F(2,2,2)=1.0
2186      F(4,2,3)=1.0
2187          F(5,5,4)=1.0
2188          F(6,5,5)=1.0
2189          F(8,5,6)=1.0
2190          F(9,8,7)=1.0
2191          F(10,8,8)=1.0
2192          F(12,8,9)=1.0
2193          F(13,8,4)=1.0
2194          F(14,8,5)=1.0
2195          F(16,8,6)=1.0
2196          L1=0.0
2197          L2=1.0
2198          L3=0.0
2199          CALL PHIXX(TRI,L1,L2,L3,G1,G2,G3,W1)
2200          CALL PHIXU(TRI,L1,L2,L3,F1,F2,F3,G1,G2,G3,W2)
2201          L1=1.0
2202          L2=0.0
2203          CALL PHIXX(TRI,L1,L2,L3,G1,G2,G3,W3)
2204          CALL PHIXU(TRI,L1,L2,L3,F1,F2,F3,G1,G2,G3,W4)
2205      L1=0.0
2206      L3=1.0
2207      CALL PHIXX(TRI,L1,L2,L3,G1,G2,G3,W5)
2208      CALL PHIXU(TRI,L1,L2,L3,F1,F2,F3,G1,G2,G3,W6)
2209      DO 180 I=1,10
2210          F(2,I,1)=W3(I)
2211          F(3,I,1)=W4(I)
2212          F(6,I,4)=W1(I)
2213          F(7,I,4)=W2(I)
2214          F(10,I,7)=W5(I)
2215          F(11,I,7)=W6(I)
2216          F(14,I,4)=W5(I)
2217          F(15,I,4)=W6(I)
2218 180      CONTINUE
2219          L1=0.0
2220          L2=1.0/3.0
2221          L3=2.0/3.0
2222          CALL PHIX(TRI,L1,L2,L3,G1,G2,G3,W1)
2223          L2=2.0/3.0
2224          L3=1.0/3.0
2225          CALL PHII(TRIP,L1,L2,L3,W2)
2226          L1=1.0/3.0
2227          L2=0.0
2228          L3=2.0/3.0
2229          CALL PHIX(TRI,L1,L2,L3,G1,G2,G3,W3)
2230          L2=2.0/3.0
2231          L3=0.0
2232          CALL PHII(TRIP,L1,L2,L3,W4)
2233          L2=1.0/3.0
2234          L3=1.0/3.0
2235          CALL PHIX(TRI,L1,L2,L3,G1,G2,G3,W5)
2236      DO 200 I=1,10
2237          DO 190 J=1,10
2238              F(17,I,J)=W1(I)*W2(J)
2239              F(19,I,J)=W5(I)*W4(J)

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2240 190          CONTINUE
2241              F(18,I,10)=W3(I)
2242              F(20,I,10)=W5(I)
2243 200          CONTINUE
2244              ENDIF
2245          ENDIF
2246
2247 * ZERO THE SB MATRIX
2248     DO 220 I=1,10
2249         DO 210 J=1,10
2250             SB(I,J)=0.0
2251 210         CONTINUE
2252 220     CONTINUE
2253
2254 * ASSEMBLE SB
2255     DO 250 K=1,20
2256         DO 240 I=1,10
2257             DO 230 J=1,10
2258                 SB(I,J)=SB(I,J)+H(2,K)*F(K,I,J)*UU(1)+H(3,K)*F(K,I,J)
2259 C                 *UU(2)+H(4,K)*F(K,I,J)*UU(3)+H(5,K)*F(K,I,J)*UU(4)
2260 230             CONTINUE
2261 240         CONTINUE
2262 250     CONTINUE
2263
2264     END
2265
2266 *****
2267
2268     SUBROUTINE PN(PHI,CORDND,SIGMAS,N,NTRIA,RANGE)
2269
2270     PARAMETER (MNODE=151 , MNTRIA=50)
2271
2272     DOUBLE PRECISION CORDND(MNODE,2),PHI(MNODE),PSI(21,9)
2273     DOUBLE PRECISION RANGE,SIGMAS,PERC,TPERC,APERC
2274     DOUBLE PRECISION ML(MNTRIA,10,10)
2275     DOUBLE PRECISION NLM(MNTRIA,16,10,10),NLI(MNTRIA,4,10)
2276     DOUBLE PRECISION MG(MNODE,MNODE)
2277     DOUBLE PRECISION GT(MNTRIA,10,10),LI(MNTRIA,10,4)
2278     INTEGER N,NTRIA,X,U
2279
2280     COMMON MG,ML,NLM,NLI,LI,GT
2281 * READ IN ARRAY OF EXACT SOLUTION - THIS DATA FILE HAS C=.5
2282 * RESULTS
2283     OPEN (18,FILE='PNDATA5',STATUS='OLD')
2284     REWIND (18)
2285     DO 100 I=1,21
2286         READ (18,5000) (PSI(I,U),U=1,9)
2287 100     CONTINUE
2288     CLOSE (18)
2289
2290 * CALCULATE PERCENT DIFFERENCE
2291     K=0
2292     TPERC=0.0
2293     PRINT*,' COORDINATES          CURRENTS          FIN ELEM'
2294     PRINT*,'          X          U          X          U          FLUX          FLUX          % DIFF'
2295     DO 200 I=1,N-NTRIA,3

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2296      IF (INT(CORDND(I,1)/.25)*.25.EQ.CORDND(I,1)) THEN
2297      X=NINT(4*CORDND(I,1)+1)
2298      U=NINT(4*CORDND(I,2)+5)
2299      PERC=100.0*ABS(PSI(X,U)-PHI(I))/PSI(X,U)
2300      WRITE (*,5001) CORDND(I,1),CORDND(I,2),PHI(I+1),PHI(I+2),
2301      C      PHI(I),PSI(X,U),PERC
2302      IF (CORDND(I,1).EQ.0.0.AND.CORDND(I,2).GE.0.0) THEN
2303      GO TO 200
2304      ELSE
2305      IF (CORDND(I,1).EQ.RANGE.AND.CORDND(I,2).LE.0.0) THEN
2306      GO TO 200
2307      ENDIF
2308      ENDIF
2309      TPERC=TPERC+PERC
2310      K=K+1
2311      ENDIF
2312      R,2399
2313      200      CONTINUE
2314      APERC=TPERC/K
2315      PRINT*, 'AVERAGE % DIFFERENCE IS ..', APERC
2316      D=NTRIA/RANGE
2317      PRINT*, 'FOR AN AVERAGE OF', D, 'TRIANGLES PER MEAN FREE PATH'
2318
2319      5000      FORMAT(2X,1P10E13.4)
2320      5001      FORMAT(6(1X,F7.3),2X,F5.2)
2321      END
EOF..
EOT..

```

```

181 ==> CO MESHE3.9 MESH
182 ==> XEF9
183 IER IS ... 0
184 NTRIA N SIGMAS
185 46 151 0.900
186 RANGE IS.... 3.000000000
187 NODAL VALUES OF THE FLUX
188 1 0.3534 2 0.3434
189 3 0.3292 4 0.3044
190 5 0.2500 6 0.1864
191 7 0.1656 8 0.1481
192 9 0.1413 10 0.2554
193 11 0.2288 12 0.1614
194 13 0.1381 14 0.1239
195 15 0.0976 16 0.0904
196 17 0.1745 18 0.1273
197 19 0.0903 20 0.0713
198 21 0.0591 22 0.1208
199 23 0.0999 24 0.0691
200 25 0.0606 26 0.0543
201 27 0.0441 28 0.0398
202 29 0.0826 30 0.0557
203 31 0.0427 32 0.0377
204 33 0.0337 34 0.0306
205 35 0.0280 36 0.2539
206 ELEMENT PENALTY VALUES
207 1 0.57885E-03 2 0.65116E-03
208 3 0.76555E-03 4 0.83027E-03
209 5 0.45322E-03 6 0.10514E-03
210 7 -.75873E-04 8 -.19484E-03
211 9 -.30669E-03 10 -.41093E-03
212 11 -.73112E-03 12 -.57047E-03
213 13 -.64482E-03 14 -.48787E-03
214 15 0.39001E-03 16 0.51147E-03
215 17 0.41353E-03 18 0.53690E-04
216 19 -.29261E-04 20 -.96223E-04
217 21 -.21822E-03 22 -.39397E-03
218 23 -.36922E-03 24 -.26522E-03
219 25 0.15227E-03 26 0.29752E-03
220 27 0.11491E-03 28 0.27448E-04
221 29 -.16711E-04 30 -.33954E-04
222 31 -.12193E-03 32 -.13218E-03

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223	33	-.20394E-03	34	-.87472E-04			
224	35	0.90719E-04	36	0.10032E-03			
225	37	0.64651E-04	38	0.57640E-05			
226	39	-.72660E-05	40	-.18721E-04			
227	41	-.12605E-04	42	-.31310E-04			
228	43	-.75572E-04	44	-.31328E-04			
229	45	-.36920E-04	46	-.48821E-04			
230	TOTAL PENALTY .... AND SUM OF ABS(PENALTY) ARE ..						
231		-.46949E-04		0.11260E-01			
232	COORDINATES		CURRENTS		FIN ELEM		
233	X	U	X	U	FLUX	FLUX	% DIFF
234	0.000	1.000	-0.111	0.984	0.353	0.353	0.00
235	0.000	0.750	-0.164	-0.297	0.343	0.343	0.00
236	0.000	0.500	-0.212	0.115	0.329	0.329	0.00
237	0.000	0.250	-0.373	0.578	0.304	0.304	0.00
238	0.000	0.000	-0.529	0.403	0.250	0.250	0.00
239	0.000	-0.250	-0.238	0.076	0.186	0.196	4.67
240	0.000	-0.500	-0.156	0.041	0.166	0.171	3.06
241	0.000	-0.750	-0.118	0.020	0.148	0.157	5.42
242	0.000	-1.000	-0.099	-0.161	0.141	0.147	3.56
243	0.750	1.000	-0.119	0.552	0.255	0.262	2.61
244	0.750	0.750	-0.141	0.045	0.229	0.236	3.12
245	0.750	0.250	-0.129	0.148	0.161	0.169	4.49
246	0.750	0.000	-0.234	0.193	0.138	0.142	2.79
247	0.750	-0.250	-0.129	0.133	0.124	0.125	0.99
248	0.750	-0.750	-0.073	0.040	0.098	0.101	3.28
249	0.750	-1.000	-0.057	-0.064	0.090	0.091	1.23
250	1.500	1.000	-0.079	0.173	0.174	0.184	5.08
251	1.500	0.500	-0.082	0.158	0.127	0.132	3.38
252	1.500	0.000	-0.116	0.090	0.090	0.095	4.52
253	1.500	-0.500	-0.058	0.043	0.071	0.075	4.52
254	1.500	-1.000	-0.038	0.020	0.059	0.062	4.35
255	2.250	1.000	-0.060	0.122	0.121	0.127	4.74
256	2.250	0.750	-0.054	0.063	0.100	0.106	5.62
257	2.250	0.250	-0.047	0.044	0.069	0.073	5.56
258	2.250	0.000	-0.094	0.075	0.061	0.063	4.46
259	2.250	-0.250	-0.052	0.066	0.054	0.056	3.07
260	2.250	-0.750	-0.030	0.032	0.044	0.045	3.03
261	2.250	-1.000	-0.022	0.039	0.040	0.042	4.30
262	3.000	1.000	-0.040	0.076	0.083	0.087	4.85
263	3.000	0.500	-0.030	0.045	0.056	0.058	4.28
264	3.000	0.000	-0.035	0.012	0.043	0.043	0.00
265	3.000	-0.250	-0.033	0.291	0.038	0.038	0.00
266	3.000	-0.500	-0.018	-0.015	0.034	0.034	0.00
267	3.000	-0.750	-0.017	0.045	0.031	0.031	0.00
268	3.000	-1.000	-0.013	0.070	0.028	0.028	0.00
269	AVERAGE % DIFFERENCE IS ..				3.877686025		
270	FOR AN AVERAGE OF 15.333				TRIANGLES PER MEAN FREE PATH		

ED C9OUT

LI,1,300

1 ==> CO MSHE3.9C MESH

2 ==> XE

3 IER IS ... 0

4 NTRIA N SIGMAS

5 46 151 0.900

6 RANGE IS.... 3.000000000

7 NODAL VALUES OF THE FLUX

8	1	0.3534	2	0.3434
9	3	0.3292	4	0.3044
10	5	0.2500	6	0.1892
11	7	0.1691	8	0.1519
12	9	0.1439	10	0.2580
13	11	0.2325	12	0.1660
14	13	0.1419	14	0.1269
15	15	0.1004	16	0.0927
16	17	0.1818	18	0.1293
17	19	0.0930	20	0.0736
18	21	0.0604	22	0.1253
19	23	0.1035	24	0.0714
20	25	0.0626	26	0.0562
21	27	0.0450	28	0.0406
22	29	0.0856	30	0.0571
23	31	0.0427	32	0.0377
24	33	0.0337	34	0.0306
25	35	0.0280	36	0.2804

26 ELEMENT PENALTY VALUES

27	1	0.69119E-03	2	0.79918E-03
28	3	0.70362E-03	4	0.79296E-03
29	5	0.40508E-03	6	0.10532E-03
30	7	-.84340E-04	8	-.19188E-03
31	9	-.30460E-03	10	-.42177E-03
32	11	-.75959E-03	12	-.58829E-03
33	13	-.66508E-03	14	-.51004E-03
34	15	0.44435E-03	16	0.54365E-03
35	17	0.40379E-03	18	0.57488E-04
36	19	-.32378E-04	20	-.10216E-03
37	21	-.23084E-03	22	-.41572E-03
38	23	-.39299E-03	24	-.28130E-03
39	25	0.16749E-03	26	0.31947E-03
40	27	0.11766E-03	28	0.30371E-04
41	29	-.17476E-04	30	-.36011E-04
42	31	-.12910E-03	32	-.14093E-03
43	33	-.22000E-03	34	-.95110E-04
44	35	0.99120E-04	36	0.10831E-03
45	37	0.67810E-04	38	0.71457E-05
46	39	-.77406E-05	40	-.20200E-04
47	41	-.18113E-04	42	-.26107E-04
48	43	-.80449E-04	44	-.35963E-04
49	45	-.40512E-04	46	-.54356E-04

50 TOTAL PENALTY .... AND SUM OF ABS(PENALTY) ARE ..

51 -.39050E-04 0.11767E-01

52 COORDINATES CURRENTS FIN ELEM

53	X	U	X	U	FLUX	FLUX	Z DIFF
54	0.000	1.000	-0.134	0.040	0.353	0.353	0.00

55	0.000	0.750	-0.160	0.049	0.343	0.343	0.00							
56	0.000	0.500	-0.227	0.078	0.329	0.329	0.00							
57	0.000	0.250	-0.357	0.158	0.304	0.304	0.00							
58	0.000	0.000	-0.489	0.218	0.250	0.250	0.00							
59	0.000	-0.250	-0.213	0.043	0.189	0.196	3.26							
60	0.000	-0.500	-0.148	0.045	0.169	0.171	1.04							
61	0.000	-0.750	-0.113	0.027	0.152	0.157	3.03							
62	0.000	-1.000	-0.097	-0.135	0.144	0.147	1.81							
63	0.750	1.000	-0.115	0.111	0.258	0.262	1.62							
64	0.750	0.750	-0.125	0.106	0.233	0.236	1.53							
65	0.750	0.250	-0.127	0.152	0.166	0.169	1.77							
66	0.750	0.000	-0.236	0.177	0.142	0.142	0.16							
67	0.750	-0.250	-0.126	0.122	0.127	0.125	1.33							
68	0.750	-0.750	-0.074	0.039	0.100	0.101	0.45							
69	0.750	-1.000	-0.058	-0.052	0.093	0.091	1.35							
70	1.500	1.000	-0.088	0.130	0.182	0.184	1.10							
71	1.500	0.500	-0.079	0.128	0.129	0.132	1.90							
72	1.500	0.000	-0.114	0.085	0.093	0.095	1.61							
73	1.500	-0.500	-0.058	0.047	0.074	0.075	1.45							
74	1.500	-1.000	-0.040	0.027	0.060	0.062	2.33							
75	2.250	1.000	-0.063	0.105	0.125	0.127	1.16							
76	2.250	0.750	-0.056	0.080	0.103	0.106	2.26							
77	2.250	0.250	-0.049	0.048	0.071	0.073	2.43							
78	2.250	0.000	-0.096	0.075	0.063	0.063	1.30							
79	2.250	-0.250	-0.050	0.052	0.056	0.056	0.29							
80	2.250	-0.750	-0.030	0.020	0.045	0.045	0.93							
81	2.250	-1.000	-0.023	0.016	0.041	0.042	2.34							
82	3.000	1.000	-0.043	0.075	0.086	0.087	1.40							
83	3.000	0.500	-0.032	0.045	0.057	0.058	1.92							
84	3.000	0.000	-0.042	0.020	0.043	0.043	0.00							
85	3.000	-0.250	-0.030	0.018	0.038	0.038	0.00							
86	3.000	-0.500	-0.024	0.014	0.034	0.034	0.00							
87	3.000	-0.750	-0.017	0.012	0.031	0.031	0.00							
88	3.000	-1.000	-0.018	0.010	0.028	0.028	0.00							
89	AVERAGE % DIFFERENCE IS ..			1.590236152										
90	FOR AN AVERAGE OF 15.333			TRIANGLES PER MEAN FREE PATH										
EOT..														
UP														

Appendix B.

The Absorbing Term (quadratic, and cubic)

The absorbing term is

$$\frac{1}{2} \int dA \, \Sigma_t^2 \phi^2 \quad (3-2)$$

Which may be written as

$$= \frac{1}{2} \underbrace{\tilde{\phi}}_{\underline{\underline{G^T}}} \underbrace{\underline{\underline{MA}}} \underbrace{\underline{\underline{G^T}}} \underbrace{\phi}_{\underline{\underline{Q}}} \quad (3-5)$$

The matrices on subsequent pages labeled as QCOABS and CCOABS (for Quadratic Coefficients Absorbing term and Cubic Coefficients) generate MA of equation (3-5) from

$$\underline{\underline{MA}} = \frac{2 A \Sigma_t^2}{6!} \underline{\underline{QCOABS}} \quad (B-1)$$

and in the cubic case from

$$\underline{\underline{MA}} = \frac{2 A \Sigma_t^2}{8!} \underline{\underline{CCOABS}} \quad (B-2)$$

where A is triangle area.

cat coabs

QCOABS

24.0	4.0	4.0	6.0	2.0	6.0
4.0	24.0	4.0	6.0	6.0	2.0
4.0	4.0	24.0	2.0	6.0	6.0
6.0	6.0	2.0	4.0	2.0	2.0
2.0	6.0	6.0	2.0	4.0	2.0
6.0	2.0	6.0	2.0	2.0	4.0

cat ccoabs

CCOABS

720.0	120.0	120.0	36.0	12.0	48.0	36.0	48.0	12.0	24.0
120.0	48.0	24.0	48.0	12.0	36.0	12.0	12.0	8.0	12.0
120.0	24.0	48.0	12.0	8.0	12.0	48.0	36.0	12.0	12.0
36.0	48.0	12.0	720.0	120.0	120.0	36.0	12.0	48.0	24.0
12.0	12.0	8.0	120.0	48.0	24.0	48.0	12.0	36.0	12.0
48.0	36.0	12.0	120.0	24.0	48.0	12.0	8.0	12.0	12.0
36.0	12.0	48.0	36.0	48.0	12.0	720.0	120.0	120.0	24.0
48.0	12.0	36.0	12.0	12.0	8.0	120.0	48.0	24.0	12.0
12.0	8.0	12.0	48.0	36.0	12.0	120.0	24.0	48.0	12.0
24.0	12.0	12.0	24.0	12.0	12.0	24.0	12.0	12.0	8.0

# Appendix C - Boundary Term (quadratic and cubic)

The boundary term (3-6) is

$$\int dA \varepsilon_{\mu} u \frac{\partial \phi}{\partial x} \phi = \varepsilon_{\mu} \int dA \mu \underline{\underline{\tilde{\varphi}}} \underline{\underline{\tilde{G}^T}} \underline{\underline{m_x}} \underline{\underline{\tilde{m}}} \underline{\underline{\tilde{G}^T}} \underline{\underline{\varphi}} \quad (3-6)$$

When  $u$  is expanded as in equation 2-3, the boundary matrix can be written as the sum of 3 matrices.

$$= \frac{1}{2} \underline{\underline{\tilde{\varphi}}} \underline{\underline{\tilde{G}^T}} \left[ \underline{\underline{M_{B1}}} + \underline{\underline{M_{B2}}} + \underline{\underline{M_{B3}}} \right] \underline{\underline{\tilde{G}^T}} \underline{\underline{\varphi}} \quad (3-10)$$

These matrices are complicated by the fact that the basis functions contain derivatives of natural co-ordinates, which are distinct for every separate triangle geometry. In the quadratic case  $\underline{\underline{m_x}}$  is given by

$$\underline{\underline{m_x}} = \begin{bmatrix} 2l_1g_1 \\ 2l_2g_2 \\ 2l_3g_3 \\ l_2g_1 + l_1g_2 \\ l_3g_2 + l_2g_3 \\ l_1g_3 + l_3g_1 \end{bmatrix} \quad (2-19)$$

the product  $\underline{\underline{m_x}} \underline{\underline{\tilde{m}}}$  for any of the three matrices results in what can be thought of as a matrix of constants, multiplied by  $g_i$ 's as appropriate. If a matrix  $\underline{\underline{D}}$  is formed of the  $g_i$ 's.

$$\underline{\underline{D}} = \begin{bmatrix} g_1 & 0 \\ g_2 & 0 \\ g_3 & 0 \\ g_1 & g_2 \\ g_2 & g_3 \\ g_3 & g_1 \end{bmatrix} \quad (C-1)$$

then this can be computed for each triangle and "overlaid" in a sense on each column of constants to produce the boundary matrix. As an example consider the matrix referred to on the next page as QCOBNDI (for Quadratic COefficients Bndry term #1). It is a 6 X 12 matrix, that when D is overlaid on, and when multiplied by  $\frac{\mu, \sum, 2A}{6!}$  produces MBI

$$\underline{\underline{MB1}} = \frac{\mu, \sum, 2A}{6!} \begin{bmatrix} 48g_1 + 0 \\ 12g_2 + 0 \\ 12g_3 + 0 \\ 6g_1 + 24g_2 \\ 6g_2 + 6g_3 \\ 24g_3 + 6g_1 \end{bmatrix} \quad \text{etc.} \quad (C-2)$$

MB2 and MB3 must be formed of course with the appropriate constants ( $\mu_2$  and  $\mu_3$ ) from the matrices labeled QCOBND2 and QCOBND3.

Boundary matrices for the cubic fit are found in an analogous manner, with 3 (10 x 20) matrices, CCOBND1, CCOBND2, and CCOBND3. In the cubic case, the derivative matrix D to be overlaid is

$$\underline{\underline{D}} = \begin{bmatrix} g_1 & 0 \\ g_1 & g_2 \\ g_1 & g_3 \\ g_2 & 0 \\ g_2 & g_3 \\ g_2 & g_1 \\ g_3 & 0 \\ g_3 & g_1 \\ g_3 & g_2 \\ g_1 & g_2 \end{bmatrix} \quad (C-3)$$

In this case row 10 must be augmented by another term. The last row of CCOBND1, CCOBND2, and CCOBND3 represent 3 each dimension (10) matrices (BR1, BR2, BR3). After is formed from

$$\underline{\underline{MB}} = \underline{\underline{MB1}} + \underline{\underline{MB2}} + \underline{\underline{MB3}} \quad (C-4)$$

if

For i=1,10

$$BR(i) = BR1(i) * u_1 + BR2(i) * u_2 + BR3(i) * u_3$$

Then

For i=1,10

$$MB(10,i) = MB(10,i) + BR(i) * 2A * \Delta t / b! \quad (C-5)$$

and the boundary matrix is now completely formed.

cat cobnd1

QCOBND1

48.0	.0	8.0	.0	8.0	.0	12.0	.0	4.0	.0	12.0	.0
12.0	.0	12.0	.0	4.0	.0	8.0	.0	4.0	.0	4.0	.0
12.0	.0	4.0	.0	12.0	.0	4.0	.0	4.0	.0	8.0	.0
6.0	24.0	6.0	4.0	2.0	4.0	4.0	6.0	2.0	2.0	2.0	6.0
6.0	6.0	2.0	6.0	6.0	2.0	2.0	4.0	2.0	2.0	4.0	2.0
24.0	6.0	4.0	2.0	4.0	6.0	6.0	2.0	2.0	2.0	6.0	4.0

% cat cobnd2

QCOBND2

12.0	.0	12.0	.0	4.0	.0	8.0	.0	4.0	.0	4.0	.0
8.0	.0	48.0	.0	8.0	.0	12.0	.0	12.0	.0	4.0	.0
4.0	.0	12.0	.0	12.0	.0	4.0	.0	8.0	.0	4.0	.0
4.0	6.0	24.0	6.0	4.0	2.0	6.0	4.0	6.0	2.0	2.0	2.0
2.0	4.0	6.0	24.0	6.0	4.0	2.0	6.0	4.0	6.0	2.0	2.0
6.0	2.0	6.0	6.0	2.0	6.0	4.0	2.0	2.0	4.0	2.0	2.0

% cat cobnd3

QCOBND3

12.0	.0	4.0	.0	12.0	.0	4.0	.0	4.0	.0	8.0	.0
4.0	.0	12.0	.0	12.0	.0	4.0	.0	8.0	.0	4.0	.0
8.0	.0	8.0	.0	48.0	.0	4.0	.0	12.0	.0	12.0	.0
2.0	6.0	6.0	2.0	6.0	6.0	2.0	2.0	4.0	2.0	2.0	4.0
4.0	2.0	4.0	6.0	24.0	6.0	2.0	2.0	6.0	4.0	6.0	2.0
6.0	4.0	2.0	4.0	6.0	24.0	2.0	2.0	2.0	6.0	4.0	6.0

cat ccobnd1

# CCOBND1

2160.	0.	360.	0.	360.	0.	108.	0.	36.	0.
144.	0.	108.	0.	144.	0.	36.	0.	72.	0.
240.	720.	96.	120.	48.	120.	96.	36.	24.	12.
72.	48.	24.	36.	24.	48.	16.	12.	24.	24.
240.	720.	48.	120.	96.	120.	24.	36.	16.	12.
24.	48.	96.	36.	72.	48.	24.	12.	24.	24.
144.	0.	108.	0.	36.	0.	360.	0.	72.	0.
144.	0.	36.	0.	24.	0.	36.	0.	36.	0.
48.	48.	24.	36.	24.	12.	48.	120.	24.	24.
24.	48.	48.	12.	24.	8.	24.	12.	16.	12.
240.	48.	96.	36.	48.	12.	96.	120.	24.	24.
72.	48.	24.	12.	24.	8.	16.	12.	24.	12.
144.	0.	36.	0.	108.	0.	36.	0.	36.	0.
24.	0.	360.	0.	144.	0.	72.	0.	36.	0.
240.	48.	48.	12.	96.	36.	24.	12.	16.	12.
24.	8.	96.	120.	72.	48.	24.	24.	24.	12.
48.	48.	24.	12.	24.	36.	48.	12.	24.	12.
24.	8.	48.	120.	24.	48.	24.	24.	16.	12.
24.	120.	12.	24.	12.	48.	24.	12.	12.	8.
12.	12.	24.	48.	12.	36.	12.	12.	8.	12.
120.	48.	24.	48.	12.	36.	12.	12.	8.	12.

% cat ccobnd2

# CCBND2

360.	.	144.	.	72.	.	144.	.	36.	.
108.	.	36.	.	36.	.	24.	.	36.	.
96.	120.	72.	48.	24.	24.	240.	48.	48.	12.
96.	36.	24.	12.	16.	12.	24.	8.	24.	12.
48.	120.	24.	48.	24.	24.	48.	48.	24.	12.
24.	36.	48.	12.	24.	12.	24.	8.	16.	12.
108.	.	144.	.	36.	.	2160.	.	360.	.
360.	.	108.	.	36.	.	144.	.	72.	.
24.	36.	24.	48.	16.	12.	240.	720.	96.	120.
48.	120.	96.	36.	24.	12.	72.	48.	24.	24.
96.	36.	72.	48.	24.	12.	240.	720.	48.	120.
96.	120.	24.	36.	16.	12.	24.	48.	24.	24.
36.	.	24.	.	36.	.	144.	.	108.	.
36.	.	360.	.	72.	.	144.	.	36.	.
48.	12.	24.	8.	24.	12.	48.	48.	24.	36.
24.	12.	48.	120.	24.	24.	24.	48.	16.	12.
24.	12.	24.	8.	16.	12.	240.	48.	96.	36.
48.	12.	96.	120.	24.	24.	72.	48.	24.	12.
12.	24.	12.	12.	8.	12.	120.	24.	48.	12.
24.	12.	48.	24.	12.	12.	36.	12.	12.	8.
48.	36.	12.	120.	24.	48.	12.	8.	12.	12.

% cat ccostr3

CCOSTR3

432.0	.0	.0	72.0	.0	144.0	.0	216.0	.0	144.0
.0	72.0	.0	.0	72.0	.0	24.0	.0	72.0	.0
24.0	.0	432.0	.0	.0	216.0	.0	144.0	.0	72.0
.0	144.0	.0							
72.0	144.0	.0	32.0	24.0	24.0	48.0	48.0	72.0	24.0
48.0	72.0	24.0	.0	48.0	24.0	24.0	8.0	32.0	4.0
24.0	8.0	144.0	144.0	.0	48.0	72.0	48.0	48.0	48.0
24.0	48.0	48.0							
216.0	144.0	.0	48.0	24.0	72.0	48.0	192.0	72.0	72.0
48.0	72.0	24.0	.0	96.0	24.0	24.0	8.0	48.0	24.0
24.0	8.0	720.0	144.0	.0	192.0	72.0	240.0	48.0	96.0
24.0	240.0	48.0							
72.0	.0	.0	72.0	.0	24.0	.0	72.0	.0	24.0
.0	432.0	.0	.0	216.0	.0	144.0	.0	72.0	.0
144.0	.0	432.0	.0	.0	72.0	.0	144.0	.0	216.0
.0	144.0	.0							
72.0	24.0	.0	48.0	24.0	24.0	8.0	96.0	24.0	24.0
8.0	216.0	144.0	.0	192.0	72.0	72.0	48.0	48.0	24.0
72.0	48.0	720.0	144.0	.0	96.0	24.0	240.0	48.0	192.0
72.0	240.0	48.0							
72.0	24.0	.0	32.0	24.0	24.0	8.0	48.0	24.0	24.0
8.0	72.0	144.0	.0	48.0	72.0	24.0	48.0	32.0	24.0
24.0	48.0	144.0	144.0	.0	48.0	24.0	48.0	48.0	48.0
72.0	48.0	48.0							
432.0	.0	.0	144.0	.0	144.0	.0	720.0	.0	144.0
.0	432.0	.0	.0	720.0	.0	144.0	.0	144.0	.0
144.0	.0	6480.0	.0	.0	720.0	.0	2160.0	.0	720.0
.0	2160.0	.0							
216.0	144.0	.0	48.0	48.0	72.0	48.0	192.0	240.0	72.0
48.0	72.0	144.0	.0	96.0	240.0	24.0	48.0	48.0	48.0
24.0	48.0	720.0	2160.0	.0	192.0	240.0	240.0	720.0	96.0
240.0	240.0	720.0							
72.0	144.0	.0	48.0	48.0	24.0	48.0	96.0	240.0	24.0
48.0	216.0	144.0	.0	192.0	240.0	72.0	48.0	48.0	48.0
72.0	48.0	720.0	2160.0	.0	96.0	240.0	240.0	720.0	192.0
240.0	240.0	720.0							
36.0	108.0	36.0	24.0	36.0	16.0	.0	48.0	96.0	36.0
.0	108.0	36.0	36.0	96.0	48.0	36.0	.0	36.0	24.0
16.0	.0	360.0	360.0	72.0	72.0	96.0	24.0	.0	96.0
72.0	24.0	.0							
36.0	12.0	36.0	12.0	36.0	12.0	36.0	12.0	120.0	120.0
120.0	120.0	48.0	48.0	24.0	48.0	24.0	8.0		

% cat ccostr2

CCOSTR2

432.0	.0	.0	216.0	.0	144.0	.0	72.0	.0	144.0
.0	432.0	.0	.0	72.0	.0	144.0	.0	216.0	.0
144.0	.0	72.0	.0	.0	72.0	.0	24.0	.0	72.0
.0	24.0	.0							
216.0	144.0	.0	192.0	72.0	72.0	48.0	48.0	24.0	72.0
48.0	720.0	144.0	.0	96.0	24.0	240.0	48.0	192.0	72.0
240.0	48.0	72.0	24.0	.0	48.0	24.0	24.0	8.0	96.0
24.0	24.0	8.0							
72.0	144.0	.0	48.0	72.0	24.0	48.0	32.0	24.0	24.0
48.0	144.0	144.0	.0	48.0	24.0	48.0	48.0	48.0	72.0
48.0	48.0	72.0	24.0	.0	32.0	24.0	24.0	8.0	48.0
24.0	24.0	8.0							
432.0	.0	.0	720.0	.0	144.0	.0	144.0	.0	144.0
.0	6480.0	.0	.0	720.0	.0	2160.0	.0	720.0	.0
2160.0	.0	432.0	.0	.0	144.0	.0	144.0	.0	720.0
.0	144.0	.0							
72.0	144.0	.0	96.0	240.0	24.0	48.0	48.0	48.0	24.0
48.0	720.0	2160.0	.0	192.0	240.0	240.0	720.0	96.0	240.0
240.0	720.0	216.0	144.0	.0	48.0	48.0	72.0	48.0	192.0
240.0	72.0	48.0							
216.0	144.0	.0	192.0	240.0	72.0	48.0	48.0	48.0	72.0
48.0	720.0	2160.0	.0	96.0	240.0	240.0	720.0	192.0	240.0
240.0	720.0	72.0	144.0	.0	48.0	48.0	24.0	48.0	96.0
240.0	24.0	48.0							
72.0	.0	.0	72.0	.0	24.0	.0	72.0	.0	24.0
.0	432.0	.0	.0	216.0	.0	144.0	.0	72.0	.0
144.0	.0	432.0	.0	.0	72.0	.0	144.0	.0	216.0
.0	144.0	.0							
72.0	24.0	.0	48.0	24.0	24.0	8.0	32.0	24.0	24.0
8.0	144.0	144.0	.0	48.0	72.0	48.0	48.0	48.0	24.0
48.0	48.0	72.0	144.0	.0	32.0	24.0	24.0	48.0	48.0
72.0	24.0	48.0							
72.0	24.0	.0	96.0	24.0	24.0	8.0	48.0	24.0	24.0
8.0	720.0	144.0	.0	192.0	72.0	240.0	48.0	96.0	24.0
240.0	48.0	216.0	144.0	.0	48.0	24.0	72.0	48.0	192.0
72.0	72.0	48.0							
36.0	36.0	108.0	48.0	36.0	96.0	.0	24.0	16.0	36.0
.0	360.0	72.0	360.0	96.0	24.0	72.0	.0	72.0	24.0
96.0	.0	108.0	36.0	36.0	36.0	16.0	24.0	.0	96.0
36.0	48.0	.0							
12.0	36.0	12.0	36.0	120.0	120.0	120.0	120.0	36.0	12.0
36.0	12.0	48.0	24.0	48.0	8.0	24.0	48.0		

% cat ccostr1

CCOSTR1

6480.0	.0	.0	720.0	.0	2160.0	.0	720.0	.0	2160.0
.0	432.0	.0	.0	144.0	.0	144.0	.0	720.0	.0
144.0	.0	432.0	.0	.0	720.0	.0	144.0	.0	144.0
.0	144.0	.0							
720.0	2160.0	.0	192.0	240.0	240.0	720.0	96.0	240.0	240.0
720.0	216.0	144.0	.0	48.0	48.0	72.0	48.0	192.0	240.0
72.0	48.0	72.0	144.0	.0	96.0	240.0	24.0	48.0	48.0
48.0	24.0	48.0							
720.0	2160.0	.0	96.0	240.0	240.0	720.0	192.0	240.0	240.0
720.0	72.0	144.0	.0	48.0	48.0	24.0	48.0	96.0	240.0
24.0	48.0	216.0	144.0	.0	192.0	240.0	72.0	48.0	48.0
48.0	72.0	48.0							
432.0	.0	.0	216.0	.0	144.0	.0	72.0	.0	144.0
.0	432.0	.0	.0	72.0	.0	144.0	.0	216.0	.0
144.0	.0	72.0	.0	.0	72.0	.0	24.0	.0	72.0
.0	24.0	.0							
144.0	144.0	.0	48.0	72.0	48.0	48.0	48.0	24.0	48.0
48.0	72.0	144.0	.0	32.0	24.0	24.0	48.0	48.0	72.0
24.0	48.0	72.0	24.0	.0	48.0	24.0	24.0	8.0	32.0
24.0	24.0	8.0							
720.0	144.0	.0	192.0	72.0	240.0	48.0	96.0	24.0	240.0
48.0	216.0	144.0	.0	48.0	24.0	72.0	48.0	192.0	72.0
72.0	48.0	72.0	24.0	.0	96.0	24.0	24.0	8.0	48.0
24.0	24.0	8.0							
432.0	.0	.0	72.0	.0	144.0	.0	216.0	.0	144.0
.0	72.0	.0	.0	72.0	.0	24.0	.0	72.0	.0
24.0	.0	432.0	.0	.0	216.0	.0	144.0	.0	72.0
.0	144.0	.0							
720.0	144.0	.0	96.0	24.0	240.0	48.0	192.0	72.0	240.0
48.0	72.0	24.0	.0	48.0	24.0	24.0	8.0	96.0	24.0
24.0	8.0	216.0	144.0	.0	192.0	72.0	72.0	48.0	48.0
24.0	72.0	48.0							
144.0	144.0	.0	48.0	24.0	48.0	48.0	48.0	72.0	48.0
48.0	72.0	24.0	.0	32.0	24.0	24.0	8.0	48.0	24.0
24.0	8.0	72.0	144.0	.0	48.0	72.0	24.0	48.0	32.0
24.0	24.0	48.0							
72.0	360.0	360.0	24.0	72.0	96.0	.0	24.0	96.0	72.0
.0	36.0	36.0	108.0	16.0	24.0	36.0	.0	36.0	48.0
96.0	.0	36.0	108.0	36.0	36.0	96.0	48.0	.0	16.0
36.0	24.0	.0							
120.0	120.0	120.0	120.0	12.0	36.0	12.0	36.0	12.0	36.0
12.0	36.0	8.0	24.0	24.0	48.0	48.0	48.0		

QCDSTR5

8.0	.0	8.0	.0	8.0	.0	4.0	.0	4.0
.0	4.0	.0	4.0	.0	4.0	.0	4.0	.0
8.0	.0	24.0	.0	16.0	.0	12.0	.0	4.0
.0	8.0	.0	12.0	.0	4.0	.0	8.0	.0
8.0	.0	16.0	.0	24.0	.0	8.0	.0	4.0
.0	12.0	.0	8.0	.0	4.0	.0	12.0	.0
4.0	4.0	12.0	4.0	8.0	4.0	6.0	2.0	2.0
2.0	4.0	2.0	6.0	2.0	2.0	2.0	4.0	2.0
4.0	4.0	8.0	12.0	12.0	8.0	4.0	6.0	2.0
2.0	6.0	4.0	4.0	6.0	2.0	2.0	6.0	4.0
4.0	4.0	4.0	8.0	4.0	12.0	2.0	4.0	2.0
2.0	2.0	6.0	2.0	4.0	2.0	2.0	2.0	6.0

% cat costr6

QCDSTR6

24.0	.0	8.0	.0	16.0	.0	4.0	.0	12.0
.0	8.0	.0	4.0	.0	12.0	.0	8.0	.0
8.0	.0	8.0	.0	8.0	.0	4.0	.0	4.0
.0	4.0	.0	4.0	.0	4.0	.0	4.0	.0
16.0	.0	8.0	.0	24.0	.0	4.0	.0	8.0
.0	12.0	.0	4.0	.0	8.0	.0	12.0	.0
4.0	12.0	4.0	4.0	4.0	8.0	2.0	2.0	2.0
6.0	2.0	4.0	2.0	2.0	2.0	6.0	2.0	4.0
8.0	4.0	4.0	4.0	12.0	4.0	2.0	2.0	4.0
2.0	6.0	2.0	2.0	2.0	4.0	2.0	6.0	2.0
12.0	8.0	4.0	4.0	8.0	12.0	2.0	2.0	6.0
4.0	4.0	6.0	2.0	2.0	6.0	4.0	4.0	6.0

% cat costr3

### QCOSTR3

16.0	.0	8.0	.0	24.0	.0	4.0	.0	8.0
.0	12.0	.0	4.0	.0	8.0	.0	12.0	.0
8.0	.0	16.0	.0	24.0	.0	8.0	.0	4.0
.0	12.0	.0	8.0	.0	4.0	.0	12.0	.0
24.0	.0	24.0	.0	96.0	.0	12.0	.0	12.0
.0	48.0	.0	12.0	.0	12.0	.0	48.0	.0
4.0	8.0	8.0	4.0	12.0	12.0	4.0	2.0	2.0
4.0	6.0	6.0	4.0	2.0	2.0	4.0	6.0	6.0
12.0	4.0	12.0	8.0	48.0	12.0	6.0	4.0	6.0
2.0	24.0	6.0	6.0	4.0	6.0	2.0	24.0	6.0
8.0	12.0	4.0	12.0	12.0	48.0	2.0	6.0	4.0
6.0	6.0	24.0	2.0	6.0	4.0	6.0	6.0	24.0

% cat costr4

### QCOSTR4

24.0	.0	16.0	.0	8.0	.0	8.0	.0	12.0
.0	4.0	.0	8.0	.0	12.0	.0	4.0	.0
16.0	.0	24.0	.0	8.0	.0	12.0	.0	8.0
.0	4.0	.0	12.0	.0	8.0	.0	4.0	.0
8.0	.0	8.0	.0	8.0	.0	4.0	.0	4.0
.0	4.0	.0	4.0	.0	4.0	.0	4.0	.0
8.0	12.0	12.0	8.0	4.0	4.0	6.0	4.0	4.0
6.0	2.0	2.0	6.0	4.0	4.0	6.0	2.0	2.0
4.0	8.0	4.0	12.0	4.0	4.0	2.0	6.0	2.0
4.0	2.0	2.0	2.0	6.0	2.0	4.0	2.0	2.0
12.0	4.0	8.0	4.0	4.0	4.0	4.0	2.0	6.0
2.0	2.0	2.0	4.0	2.0	6.0	2.0	2.0	2.0

% cat costr1

QCOSTR1

96.0	.0	24.0	.0	24.0	.0	12.0	.0	48.0
.0	12.0	.0	12.0	.0	48.0	.0	12.0	.0
24.0	.0	16.0	.0	8.0	.0	8.0	.0	12.0
.0	4.0	.0	8.0	.0	12.0	.0	4.0	.0
24.0	.0	8.0	.0	16.0	.0	4.0	.0	12.0
.0	8.0	.0	4.0	.0	12.0	.0	8.0	.0
12.0	48.0	8.0	12.0	4.0	12.0	4.0	6.0	6.0
24.0	2.0	6.0	4.0	6.0	6.0	24.0	2.0	6.0
12.0	12.0	4.0	8.0	8.0	4.0	2.0	4.0	6.0
6.0	4.0	2.0	2.0	4.0	6.0	6.0	4.0	2.0
48.0	12.0	12.0	4.0	12.0	8.0	6.0	2.0	24.0
6.0	6.0	4.0	6.0	2.0	24.0	6.0	6.0	4.0

% cat costr2

QCOSTR2

16.0	.0	24.0	.0	8.0	.0	12.0	.0	8.0
.0	4.0	.0	12.0	.0	8.0	.0	4.0	.0
24.0	.0	96.0	.0	24.0	.0	48.0	.0	12.0
.0	12.0	.0	48.0	.0	12.0	.0	12.0	.0
8.0	.0	24.0	.0	16.0	.0	12.0	.0	4.0
.0	8.0	.0	12.0	.0	4.0	.0	8.0	.0
12.0	8.0	48.0	12.0	12.0	4.0	24.0	6.0	6.0
4.0	6.0	2.0	24.0	6.0	6.0	4.0	6.0	2.0
4.0	12.0	12.0	48.0	8.0	12.0	6.0	24.0	2.0
6.0	4.0	6.0	6.0	24.0	2.0	6.0	4.0	6.0
8.0	4.0	12.0	12.0	4.0	8.0	6.0	6.0	4.0
2.0	2.0	4.0	6.0	6.0	4.0	2.0	2.0	4.0

column 9

$g_1 g_3$	0	$g_1 g_2$	0
$g_1 g_3$	$g_2 g_3$	$g_1 g_2$	$g_2^2$
$g_1 g_3$	$g_3^2$	$g_1 g_2$	$g_2 g_3$
$g_3 g_2$	0	$g_2^2$	0
$g_3 g_2$	$g_3^2$	$g_2^2$	$g_3 g_2$
$g_3 g_2$	$g_3 g_1$	$g_2^2$	$g_1 g_2$
$g_3^2$	0	$g_2 g_3$	0
$g_3^2$	$g_3 g_1$	$g_2 g_3$	$g_1 g_2$
$g_3^2$	$g_2 g_3$	$g_2 g_3$	$g_2^2$
$g_1 g_3$	$g_2 g_3$	$g_3^2$	0

Figure D-2  
(continued)

column 5				column 6			
$g_1 g_2$	0	$g_1 g_3$	0	$g_1 g_2$	0	$g_1^2$	0
$g_1 g_2$	$g_2^2$	$g_1 g_3$	$g_2 g_3$	$g_1 g_2$	$g_2^2$	$g_1^2$	$g_1 g_2$
$g_1 g_2$	$g_2 g_3$	$g_1 g_3$	$g_3^2$	$g_1 g_2$	$g_2 g_3$	$g_1^2$	$g_1 g_3$
$g_2^2$	0	$g_2 g_3$	0	$g_2^2$	0	$g_1 g_2$	0
$g_2^2$	$g_2 g_3$	$g_2 g_3$	$g_3^2$	$g_2^2$	$g_2 g_3$	$g_1 g_2$	$g_1 g_3$
$g_2^2$	$g_1 g_2$	$g_2 g_3$	$g_1 g_3$	$g_2^2$	$g_1 g_2$	$g_1 g_2$	$g_1^2$
$g_2 g_3$	0	$g_3^2$	0	$g_2 g_3$	0	$g_1 g_3$	0
$g_2 g_3$	$g_1 g_2$	$g_3^2$	$g_1 g_3$	$g_2 g_3$	$g_1 g_2$	$g_1 g_3$	$g_1^2$
$g_2 g_3$	$g_2^2$	$g_3^2$	$g_2 g_3$	$g_2 g_3$	$g_2^2$	$g_1 g_3$	$g_1 g_2$
$g_1 g_2$	$g_2^2$	$g_2 g_3$	0	$g_1 g_2$	$g_2^2$	$g_2 g_3$	0

column 7				column 8			
$g_1 g_3$	0	0	0	$g_1 g_3$	0	$g_1^2$	0
$g_1 g_3$	$g_2 g_3$	0	0	$g_1 g_3$	$g_2 g_3$	$g_1^2$	$g_1 g_2$
$g_1 g_3$	$g_3^2$	0	0	$g_1 g_3$	$g_3^2$	$g_1^2$	$g_1 g_3$
$g_2 g_3$	0	0	0	$g_2 g_3$	0	$g_1 g_2$	0
$g_2 g_3$	$g_3^2$	0	0	$g_2 g_3$	$g_3^2$	$g_1 g_2$	$g_1 g_3$
$g_2 g_3$	$g_1 g_3$	0	0	$g_2 g_3$	$g_1 g_3$	$g_1 g_2$	$g_1^2$
$g_3^2$	0	0	0	$g_3^2$	0	$g_1 g_3$	0
$g_3^2$	$g_1 g_3$	0	0	$g_3^2$	$g_1 g_3$	$g_1 g_3$	$g_1^2$
$g_3^2$	$g_2 g_3$	0	0	$g_3^2$	$g_2 g_3$	$g_1 g_3$	$g_1 g_2$
$g_1 g_3$	$g_2 g_3$	$g_3^2$	0	$g_1 g_3$	$g_2 g_3$	$g_3^2$	0

Figure D-2  
(continued)

column 1				column 2			
$q_1^2$	0	0		$q_1^2$	$q_1 q_2$		
$q_1^2$	$q_1 q_2$	0		$q_1^2$	$q_1 q_2$	$q_1 q_2$	$q_2^2$
$q_1^2$	$q_1 q_3$	0		$q_1^2$	$q_1 q_3$	$q_1 q_2$	$q_2 q_3$
$q_1 q_2$	0	0		$q_1 q_2$	0	$q_2^2$	0
$q_1 q_2$	$q_1 q_3$	0		$q_1 q_2$	$q_1 q_3$	$q_2^2$	$q_2 q_3$
$q_1 q_2$	$q_1^2$	0		$q_1 q_2$	$q_1^2$	$q_2^2$	$q_1 q_2$
$q_1 q_3$	0	0		$q_1 q_3$	0	$q_2 q_3$	0
$q_1 q_3$	$q_1^2$	0		$q_1 q_3$	$q_1^2$	$q_2 q_3$	$q_1 q_2$
$q_1 q_3$	$q_1 q_2$	0		$q_1 q_3$	$q_1 q_2$	$q_2 q_3$	$q_2^2$
$q_1^2$	$q_1 q_2$	$q_1 q_3$		$q_1^2$	$q_1 q_2$	$q_1 q_3$	0

column 3				column 4			
$q_1^2$	$q_1 q_3$	0	0	$q_1 q_2$	0	0	
$q_1^2$	$q_1 q_2$	$q_1 q_3$	$q_2 q_3$	$q_1 q_2$	$q_2^2$	0	
$q_1^2$	$q_1 q_3$	$q_1 q_3$	$q_3^2$	$q_1 q_2$	$q_2 q_3$	0	
$q_1 q_2$	$q_2 q_3$	0	0	$q_2^2$	0	0	
$q_1 q_2$	$q_1 q_3$	$q_2 q_3$	$q_3^2$	$q_2^2$	$q_2 q_3$	0	
$q_1 q_2$	$q_1^2$	$q_2 q_3$	$q_1 q_3$	$q_2^2$	$q_1 q_2$	0	
$q_1 q_3$	$q_3^2$	0	0	$q_2 q_3$	0	0	
$q_1 q_3$	$q_1^2$	$q_3^2$	$q_1 q_3$	$q_2 q_3$	$q_1 q_2$	0	
$q_1 q_3$	$q_1 q_2$	$q_3^2$	$q_2 q_3$	$q_2 q_3$	$q_2^2$	0	
$q_1^2$	$q_1 q_2$	$q_1 q_3$	0	$q_1 q_2$	$q_2^2$	$q_2 q_3$	

Figure D-2  
Overlaid Matrix of Derivatives For Streaming Matrix  
with Cubic Fit

$$DS = \begin{bmatrix} \text{column 1} & \text{column 2} & \text{column 3} & \text{column 4} \\ g_1 & 0 & g_1 & 0 & g_1 & 0 & g_1^2 & 0 & g_1 g_2 & 0 \\ g_2 & 0 & g_2 & 0 & g_2 & 0 & g_2 g_1 & 0 & g_2^2 & 0 \\ g_3 & 0 & g_3 & 0 & g_3 & 0 & g_3 g_1 & 0 & g_3 g_2 & 0 \\ g_1 & g_1 g_2 & g_1 & g_2^2 & g_1 & g_2 g_3 & g_1^2 & g_2^2 & g_1^2 & g_2^2 \\ g_2 & g_1 g_3 & g_2 & g_2 g_3 & g_2 & g_3^2 & g_2 g_1 & g_3 g_3 & g_2^2 & g_2 g_3 \\ g_3 & g_1^2 & g_3 & g_1 g_2 & g_3 & g_1 g_3 & g_3 g_1 & g_1^2 & g_2 g_3 & g_1 g_2 \end{bmatrix}$$

$$\begin{bmatrix} \text{column 5} & \text{column 6} \\ g_1 g_2 & 0 & g_1 g_3 & 0 & g_1 g_3 & 0 & g_1^2 & 0 \\ g_2^2 & 0 & g_2 g_3 & 0 & g_2 g_3 & 0 & g_1 g_2 & 0 \\ g_2 g_3 & 0 & g_3^2 & 0 & g_3^2 & 0 & g_1 g_3 & 0 \\ g_1 g_2 & g_2^2 & g_1 g_3 & g_2 g_3 & g_1 g_3 & g_2 g_3 & g_1^2 & g_1 g_2 \\ g_2^2 & g_2 g_3 & g_2 g_3 & g_3^2 & g_2 g_3 & g_3^2 & g_1 g_2 & g_1 g_3 \\ g_2 g_3 & g_1 g_2 & g_3^2 & g_1 g_3 & g_3^2 & g_1 g_3 & g_1 g_3 & g_1^2 \end{bmatrix}$$

Figure D-1  
Overlaid Matrix of Derivatives For Streaming  
Matrix with Quadratic Fit

Column 10 of the streaming matrix is found by noting that it is the transpose of row ten.

with groups of 2 or 3 columns at a time, as divided by dotted lines on fig C-1, until all 10 columns of the streaming matrix are assembled.

In the cubic case, the arrays listed as CCOSTRI, CCOSTR2, ..., CCOSTR6 represent 10 x 33 matrices of constants, for rows 1 through 9 of the 6 streaming matrices with a (1 X 18) row matrix below to augment row 10 terms. DS is a 10 x 33 matrix of , which when overlayed on the sum of CCOSTRI thru 6, multiplied by the appropriate U 'S and ( ) from the integration, forms the streaming matrix.

Column 1-3 of DS overlayed on columns 1-3 of the COSTR sum produce the first column of MS. Subsequent columns of the streaming matrix are found by the next 3 or 4 columns of DS, overlayed on the corresponding CCOSTR columns, as separated by the dotted lines in DS of figure c-2.

Row 10 of the streaming matrices must be augmented by the dimension (18) matrix (SRI,SR2,...,SR6) on the last two lines of COSTR, such that

For  $i=1,18$

$$SR(i) = [u_1^2 SR1(i) + u_2^2 SR2(i) + u_3^2 SR3(i) + 2u_1 u_2 SR4(i) + 2u_2 u_3 SR5(i) + 2u_1 u_3 SR6(i)] + 2A/q!$$

AND

$$\begin{aligned} MS(10,2) &= MS(10,2) + SR(1)q_2^2 + SR(2)q_2q_3 \\ MS(10,3) &= MS(10,3) + SR(3)q_2q_3 + SR(4)q_3^2 \\ MS(10,5) &= MS(10,5) + SR(5)q_1q_3 + SR(6)q_3^2 \\ MS(10,6) &= MS(10,6) + SR(7)q_1^2 + SR(8)q_1q_3 \\ MS(10,8) &= MS(10,8) + SR(9)q_1^2 + SR(10)q_1q_2 \\ MS(10,9) &= MS(10,9) + SR(11)q_1q_2 + SR(12)q_2^2 \\ MS(10,10) &= SR(13)q_1^2 + SR(14)q_1q_2 + SR(15)q_1q_3 + SR(16)q_2^2 \\ &\quad + SR(17)q_2q_3 + SR(18)q_3^2 \end{aligned}$$

# Appendix D - The Streaming Term (quadratic and cubic)

The Streaming term is

$$\frac{1}{2} \int dA \left( u \frac{\partial \phi}{\partial x} \right)^2 \quad (D-1)$$

which can be written as the sum of 6 distinct matrices

$$\begin{aligned} &= \frac{1}{2} \underline{\underline{\phi}} \underline{\underline{G}}^T \left[ \underline{\underline{MS1}} + \underline{\underline{MS2}} + \underline{\underline{MS3}} + \underline{\underline{MS4}} + \underline{\underline{MS5}} + \underline{\underline{MS6}} \right] \underline{\underline{G}}^T \underline{\underline{\phi}} \\ &= \frac{1}{2} \underline{\underline{\phi}} \underline{\underline{G}}^T \underline{\underline{MS}} \underline{\underline{G}}^T \underline{\underline{\phi}} \end{aligned} \quad (3-13)$$

Evaluating these matrices involves taking the product  $\underline{\underline{m}}_i \underline{\underline{\tilde{m}}}_i$  which results in cross products of the natural coordinates derivatives with respect to cartesian coordinates. The six streaming matrices, as in the boundary case (Appendix C) can be thought of as distinct matrices of constants, which after being multiplied respectively by  $\mu_1^2$ ,  $\mu_2^2$ ,  $\mu_3^2$ ,  $2\mu_1\mu_2$ ,  $2\mu_2\mu_3$  and  $2\mu_1\mu_3$  can be summed, and then "overlayed" by a matrix of  $g_i^j$ 's. Due to the cross products, this matrix of derivatives ( $\underline{\underline{DS}}$ ) is complicated. It is generated in Subroutine Stream, (appendix A) for the cubic case, and written out below for both the quadratic and cubic cases.

DS for the quadratic case is listed in figure d-1. After multiplying the 6 QCOSTR matrices by the appropriate u values; and a factor of  $(2^A/6!)$  from the integration, they may be summed to form a single 6x18 matrix. The first two columns of this matrix overlay on the first two columns of DS to form the first column of the streaming matrix. The process continues

% cat ccoabnd3

CCOABND3

360.	.	72.	.	144.	.	36.	.	24.	.
36.	.	144.	.	108.	.	36.	.	36.	.
48.	120.	24.	24.	24.	48.	48.	12.	24.	8.
24.	12.	48.	48.	24.	36.	24.	12.	16.	12.
96.	120.	24.	24.	72.	48.	24.	12.	24.	8.
16.	12.	240.	48.	96.	36.	48.	12.	24.	12.
36.	.	36.	.	24.	.	360.	.	144.	.
72.	.	144.	.	36.	.	108.	.	36.	.
24.	12.	16.	12.	24.	8.	96.	120.	72.	48.
24.	24.	240.	48.	48.	12.	96.	36.	24.	12.
48.	12.	24.	12.	24.	8.	48.	120.	24.	48.
24.	24.	48.	48.	24.	12.	24.	36.	16.	12.
108.	.	36.	.	144.	.	108.	.	144.	.
36.	.	2160.	.	360.	.	360.	.	72.	.
96.	36.	24.	12.	72.	48.	24.	36.	24.	48.
16.	12.	240.	720.	96.	120.	48.	120.	24.	24.
24.	36.	16.	12.	24.	48.	96.	36.	72.	48.
24.	12.	240.	720.	48.	120.	96.	120.	24.	24.
12.	48.	8.	12.	12.	36.	48.	12.	36.	12.
12.	8.	120.	120.	24.	48.	48.	24.	12.	12.
24.	12.	12.	24.	12.	12.	24.	12.	12.	8.

% cat ccostr4

CCOSTR4

1080.0	.0	.0	288.0	.0	360.0	.0	144.0	.0	360.0
.0	324.0	.0	.0	72.0	.0	108.0	.0	288.0	.0
108.0	.0	108.0	.0	.0	144.0	.0	36.0	.0	72.0
.0	36.0	.0							
288.0	360.0	.0	144.0	96.0	96.0	120.0	48.0	48.0	96.0
120.0	288.0	108.0	.0	48.0	24.0	96.0	36.0	144.0	96.0
96.0	36.0	48.0	36.0	.0	48.0	48.0	16.0	12.0	48.0
24.0	16.0	12.0							
144.0	360.0	.0	48.0	96.0	48.0	120.0	48.0	48.0	48.0
120.0	72.0	108.0	.0	32.0	24.0	24.0	36.0	48.0	96.0
24.0	36.0	72.0	36.0	.0	48.0	48.0	24.0	12.0	32.0
24.0	24.0	12.0							
324.0	.0	.0	288.0	.0	108.0	.0	72.0	.0	108.0
.0	1080.0	.0	.0	144.0	.0	360.0	.0	288.0	.0
360.0	.0	108.0	.0	.0	72.0	.0	36.0	.0	144.0
.0	36.0	.0							
72.0	108.0	.0	48.0	96.0	24.0	36.0	32.0	24.0	24.0
36.0	144.0	360.0	.0	48.0	48.0	48.0	120.0	48.0	96.0
48.0	120.0	72.0	36.0	.0	32.0	24.0	24.0	12.0	48.0
48.0	24.0	12.0							
288.0	108.0	.0	144.0	96.0	96.0	36.0	48.0	24.0	96.0
36.0	288.0	360.0	.0	48.0	48.0	96.0	120.0	144.0	96.0
96.0	120.0	48.0	36.0	.0	48.0	24.0	16.0	12.0	48.0
48.0	16.0	12.0							
108.0	.0	.0	48.0	.0	36.0	.0	72.0	.0	36.0
.0	108.0	.0	.0	72.0	.0	36.0	.0	48.0	.0
36.0	.0	216.0	.0	.0	72.0	.0	72.0	.0	72.0
.0	72.0	.0							
144.0	36.0	.0	48.0	16.0	48.0	12.0	48.0	24.0	48.0
12.0	72.0	36.0	.0	32.0	24.0	24.0	12.0	48.0	16.0
24.0	12.0	72.0	72.0	.0	48.0	24.0	24.0	24.0	32.0
24.0	24.0	24.0							
72.0	36.0	.0	48.0	16.0	24.0	12.0	32.0	24.0	24.0
12.0	144.0	36.0	.0	48.0	24.0	48.0	12.0	48.0	16.0
48.0	12.0	72.0	72.0	.0	32.0	24.0	24.0	24.0	48.0
24.0	24.0	24.0							
36.0	72.0	144.0	24.0	36.0	72.0	.0	16.0	24.0	36.0
.0	72.0	36.0	144.0	24.0	16.0	36.0	.0	36.0	24.0
72.0	.0	36.0	36.0	24.0	24.0	24.0	24.0	.0	24.0
24.0	24.0	.0							
24.0	48.0	24.0	48.0	24.0	48.0	24.0	48.0	12.0	12.0
12.0	12.0	12.0	16.0	24.0	12.0	24.0	36.0		

% cat ccostr5

CCOSTR5

216.0	.0	.0	72.0	.0	72.0	.0	72.0	.0	72.0
.0	108.0	.0	.0	48.0	.0	36.0	.0	72.0	.0
36.0	.0	108.0	.0	.0	72.0	.0	36.0	.0	48.0
.0	36.0	.0							
72.0	72.0	.0	48.0	24.0	24.0	24.0	32.0	24.0	24.0
24.0	144.0	36.0	.0	48.0	16.0	48.0	12.0	48.0	24.0
48.0	12.0	72.0	36.0	.0	32.0	24.0	24.0	12.0	48.0
16.0	24.0	12.0							
72.0	72.0	.0	32.0	24.0	24.0	24.0	48.0	24.0	24.0
24.0	72.0	36.0	.0	48.0	16.0	24.0	12.0	32.0	24.0
24.0	12.0	144.0	36.0	.0	48.0	24.0	48.0	12.0	48.0
16.0	48.0	12.0							
108.0	.0	.0	144.0	.0	36.0	.0	72.0	.0	36.0
.0	1080.0	.0	.0	288.0	.0	360.0	.0	144.0	.0
360.0	.0	324.0	.0	.0	72.0	.0	108.0	.0	288.0
.0	108.0	.0							
48.0	36.0	.0	48.0	48.0	16.0	12.0	48.0	24.0	16.0
12.0	288.0	360.0	.0	144.0	96.0	96.0	120.0	48.0	48.0
96.0	120.0	288.0	108.0	.0	48.0	24.0	96.0	36.0	144.0
96.0	96.0	36.0							
72.0	36.0	.0	48.0	48.0	24.0	12.0	32.0	24.0	24.0
12.0	144.0	360.0	.0	48.0	96.0	48.0	120.0	48.0	48.0
48.0	120.0	72.0	108.0	.0	32.0	24.0	24.0	36.0	48.0
96.0	24.0	36.0							
108.0	.0	.0	72.0	.0	36.0	.0	144.0	.0	36.0
.0	324.0	.0	.0	288.0	.0	108.0	.0	72.0	.0
108.0	.0	1080.0	.0	.0	144.0	.0	360.0	.0	288.0
.0	360.0	.0							
72.0	36.0	.0	32.0	24.0	24.0	12.0	48.0	48.0	24.0
12.0	72.0	108.0	.0	48.0	96.0	24.0	36.0	32.0	24.0
24.0	36.0	144.0	360.0	.0	48.0	48.0	48.0	120.0	48.0
96.0	48.0	120.0							
48.0	36.0	.0	48.0	24.0	16.0	12.0	48.0	48.0	16.0
12.0	288.0	108.0	.0	144.0	96.0	96.0	36.0	48.0	24.0
96.0	36.0	288.0	360.0	.0	48.0	48.0	96.0	120.0	144.0
96.0	96.0	120.0							
24.0	36.0	36.0	24.0	24.0	24.0	.0	24.0	24.0	24.0
.0	144.0	36.0	72.0	72.0	24.0	36.0	.0	36.0	16.0
24.0	.0	144.0	72.0	36.0	36.0	24.0	16.0	.0	72.0
36.0	24.0	.0							
12.0	12.0	12.0	12.0	48.0	24.0	48.0	24.0	48.0	24.0
48.0	24.0	36.0	24.0	24.0	12.0	16.0	12.0		

% cat ccostr6

CCOSTR6

1080.0	.0	.0	144.0	.0	360.0	.0	288.0	.0	360.0
.0	108.0	.0	.0	72.0	.0	36.0	.0	144.0	.0
36.0	.0	324.0	.0	.0	288.0	.0	108.0	.0	72.0
.0	108.0	.0							
144.0	360.0	.0	48.0	48.0	48.0	120.0	48.0	96.0	48.0
120.0	72.0	36.0	.0	32.0	24.0	24.0	12.0	48.0	48.0
24.0	12.0	72.0	108.0	.0	48.0	96.0	24.0	36.0	32.0
24.0	24.0	36.0							
288.0	360.0	.0	48.0	48.0	96.0	120.0	144.0	96.0	96.0
120.0	48.0	36.0	.0	48.0	24.0	16.0	12.0	48.0	48.0
16.0	12.0	288.0	108.0	.0	144.0	96.0	96.0	36.0	48.0
24.0	96.0	36.0							
108.0	.0	.0	72.0	.0	36.0	.0	48.0	.0	36.0
.0	216.0	.0	.0	72.0	.0	72.0	.0	72.0	.0
72.0	.0	108.0	.0	.0	48.0	.0	36.0	.0	72.0
.0	36.0	.0							
72.0	36.0	.0	32.0	24.0	24.0	12.0	48.0	16.0	24.0
12.0	72.0	72.0	.0	48.0	24.0	24.0	24.0	32.0	24.0
24.0	24.0	144.0	36.0	.0	48.0	16.0	48.0	12.0	48.0
24.0	48.0	12.0							
144.0	36.0	.0	48.0	24.0	48.0	12.0	48.0	16.0	48.0
12.0	72.0	72.0	.0	32.0	24.0	24.0	24.0	48.0	24.0
24.0	24.0	72.0	36.0	.0	48.0	16.0	24.0	12.0	32.0
24.0	24.0	12.0							
324.0	.0	.0	72.0	.0	108.0	.0	288.0	.0	108.0
.0	108.0	.0	.0	144.0	.0	36.0	.0	72.0	.0
36.0	.0	1080.0	.0	.0	288.0	.0	360.0	.0	144.0
.0	360.0	.0							
288.0	108.0	.0	48.0	24.0	96.0	36.0	144.0	96.0	96.0
36.0	48.0	36.0	.0	48.0	48.0	16.0	12.0	48.0	24.0
16.0	12.0	288.0	360.0	.0	144.0	96.0	96.0	120.0	48.0
48.0	96.0	120.0							
72.0	108.0	.0	32.0	24.0	24.0	36.0	48.0	96.0	24.0
36.0	72.0	36.0	.0	48.0	48.0	24.0	12.0	32.0	24.0
24.0	12.0	144.0	360.0	.0	48.0	96.0	48.0	120.0	48.0
48.0	48.0	120.0							
36.0	144.0	72.0	16.0	36.0	24.0	.0	24.0	72.0	36.0
.0	36.0	24.0	36.0	24.0	24.0	24.0	.0	24.0	24.0
24.0	.0	72.0	144.0	36.0	36.0	72.0	24.0	.0	24.0
36.0	16.0	.0							
48.0	24.0	48.0	24.0	12.0	12.0	12.0	12.0	24.0	48.0
24.0	48.0	12.0	24.0	16.0	36.0	24.0	12.0		

# Appendix E - The Scattering Integrals

The first scattering integral is

$$\iiint dx du du' \propto \phi \phi' \quad (4-3)$$

where  $\alpha = \frac{\Sigma_s^2}{2} - \Sigma_t \Sigma_s$ . If the product  $\phi \phi' = F$ , then a cubic can be specified over the tetrahedron using the twenty degrees of freedom specified in figure 2-6. Consider case 1 as depicted in figure 4-4.

$$F = \begin{bmatrix} \varphi_2 \varphi_1' & \varphi_{2x} \varphi_1' + \varphi_2 \varphi_{1x}' & \varphi_{2u} \varphi_1' & \varphi_2 \varphi_{1u}' \\ \varphi_1 \varphi_3' & \varphi_{1x} \varphi_3' + \varphi_1 \varphi_{3x}' & \varphi_{1u} \varphi_3' & \varphi_1 \varphi_{3u}' \\ \varphi_3 \varphi_1' & \varphi_{3x} \varphi_1' + \varphi_3 \varphi_{1x}' & \varphi_{3u} \varphi_1' & \varphi_3 \varphi_{1u}' \\ \varphi_1 \varphi_2' & \varphi_{1x} \varphi_2' + \varphi_1 \varphi_{2x}' & \varphi_{1u} \varphi_2' & \varphi_1 \varphi_{2u}' \\ \varphi_{12} \varphi_{10}' & \varphi_{10} \varphi_{14} & \varphi_{11} \varphi_{10}' & \varphi_{10} \varphi_{13}' \end{bmatrix} \quad (E-1)$$

points 11 and 12 are on the local triangle at  $(\frac{2}{3}, \frac{1}{3}, 0)$  and  $(\frac{2}{3}, 0, \frac{1}{3})$  respectively and 13 and 14 are on the non local triangle at  $(\frac{2}{3}, 0, \frac{1}{3})$  and  $(\frac{2}{3}, \frac{1}{3}, 0)$  respectively. It should be noted that these are not finite element interpolation nodes, but that they can be written in terms of these nodes using (2-13). The second scattering integral is

$$\iiint dx du du' (-\Sigma_s) u \frac{\partial \phi}{\partial x} \phi' \quad (4-3)$$

If  $G = \frac{\partial \phi}{\partial x} \phi'$ , then the twenty degrees of freedom for case 1 are

$$\underline{G} = \begin{bmatrix} \varphi_{2x} \varphi'_1 & \varphi_{2xx} \varphi'_1 + \varphi_{2x} \varphi'_{1x} & \varphi_{2ux} \varphi'_1 & \varphi_{2x} \varphi'_{1u} \\ \varphi_{1x} \varphi'_3 & \varphi_{1xx} \varphi'_3 + \varphi_{1x} \varphi'_{3x} & \varphi_{1ux} \varphi'_3 & \varphi_{1x} \varphi'_{3u} \\ \varphi_{3x} \varphi'_1 & \varphi_{3xx} \varphi'_1 + \varphi_{3x} \varphi'_{1x} & \varphi_{3ux} \varphi'_1 & \varphi_{3x} \varphi'_{1u} \\ \varphi_{1x} \varphi'_2 & \varphi_{1xx} \varphi'_2 + \varphi_{1x} \varphi'_{2x} & \varphi_{1ux} \varphi'_2 & \varphi_{1x} \varphi'_{2u} \\ \varphi_{12x} \varphi'_{10} & \varphi_{10x} \varphi'_{14} & \varphi_{11x} \varphi'_{10} & \varphi_{10x} \varphi'_{13} \end{bmatrix} \quad (E-2)$$

For case 3

$$\underline{F} = \begin{bmatrix} \varphi_2 \varphi'_1 & \varphi_{2x} \varphi'_1 + \varphi_2 \varphi'_{1x} & \varphi_{2u} \varphi'_1 & \varphi_2 \varphi'_{1u} \\ \varphi_3 \varphi'_1 & \varphi_{3x} \varphi'_1 + \varphi_3 \varphi'_{1x} & \varphi_{3u} \varphi'_1 & \varphi_3 \varphi'_{1u} \\ \varphi_1 \varphi'_3 & \varphi_{1x} \varphi'_3 + \varphi_1 \varphi'_{3x} & \varphi_{1u} \varphi'_3 & \varphi_{1x} \varphi'_{3u} \\ \varphi_1 \varphi'_2 & \varphi_{1x} \varphi'_2 + \varphi_1 \varphi'_{2x} & \varphi_{1u} \varphi'_2 & \varphi_1 \varphi'_{2u} \\ \varphi_{11} \varphi'_{10} & \varphi_{12} \varphi'_{10} & \varphi_{10} \varphi'_{13} & \varphi_{10} \varphi'_{14} \end{bmatrix} \quad (E-3)$$

and

$$\underline{G} = \begin{bmatrix} \varphi_{2x} \varphi'_1 & \varphi_{2xx} \varphi'_1 + \varphi_{2x} \varphi'_{1x} & \varphi_{2ux} \varphi'_1 & \varphi_{2x} \varphi'_{1u} \\ \varphi_{3x} \varphi'_1 & \varphi_{3xx} \varphi'_1 + \varphi_{3x} \varphi'_{1x} & \varphi_{3ux} \varphi'_1 & \varphi_{3x} \varphi'_{1u} \\ \varphi_{1x} \varphi'_3 & \varphi_{1xx} \varphi'_3 + \varphi_{1x} \varphi'_{3x} & \varphi_{1ux} \varphi'_3 & \varphi_{1x} \varphi'_{3u} \\ \varphi_{1x} \varphi'_2 & \varphi_{1xx} \varphi'_2 + \varphi_{1x} \varphi'_{2x} & \varphi_{1ux} \varphi'_2 & \varphi_{1x} \varphi'_{2u} \\ \varphi_{11x} \varphi'_{10} & \varphi_{12x} \varphi'_{10} & \varphi_{10x} \varphi'_{13} & \varphi_{10x} \varphi'_{14} \end{bmatrix} \quad (E-4)$$

where  $\varphi_{11}$  and  $\varphi_{12}$  are on the local triangle at  $(\frac{2}{3}, 0, \frac{1}{3})$  and  $(\frac{2}{3}, \frac{1}{3}, 0)$  respectively. Points 13 and 14 are non local at  $(\frac{2}{3}, \frac{1}{3}, 0)$  and  $(\frac{2}{3}, 0, \frac{1}{3})$ .

Continuing to number as in figure 4-4, the integrals for case 2 and case 4 must be done separately over the two halves and summed. Case 2, the left half is

$$F = \begin{bmatrix} \psi_1 \psi_1' & \psi_{1x} \psi_1' + \psi_1 \psi_{1x}' & \psi_{1u} \psi_1' & \psi_1 \psi_{1u}' \\ \psi_3 \psi_3' & \psi_{3x} \psi_3' + \psi_3 \psi_{3x}' & \psi_{3u} \psi_3' & \psi_3 \psi_{3u}' \\ \psi_2 \psi_2' & \psi_{2x} \psi_2' + \psi_2 \psi_{2x}' & \psi_{2u} \psi_2' & \psi_2 \psi_{2u}' \\ \psi_3 \psi_2' & \psi_{3x} \psi_2' + \psi_3 \psi_{2x}' & \psi_{3u} \psi_2' & \psi_3 \psi_{2u}' \\ \psi_{15} \psi_{18} & \psi_{10} \psi_{14} & \psi_{11} \psi_{10}' & \psi_{10} \psi_{10}' \end{bmatrix} \quad (E-5)$$

and

$$G = \begin{bmatrix} \psi_{1x} \psi_1' & \psi_{1xx} \psi_1' + \psi_{1x} \psi_{1x}' & \psi_{1ux} \psi_1' & \psi_{1x} \psi_{1u}' \\ \psi_{3x} \psi_3' & \psi_{3xx} \psi_3' + \psi_{3x} \psi_{3x}' & \psi_{3ux} \psi_3' & \psi_{3x} \psi_{3u}' \\ \psi_{2x} \psi_2' & \psi_{2xx} \psi_2' + \psi_{2x} \psi_{2x}' & \psi_{2ux} \psi_2' & \psi_{2x} \psi_{2u}' \\ \psi_{3x} \psi_2' & \psi_{3xx} \psi_2' + \psi_{3x} \psi_{2x}' & \psi_{3ux} \psi_2' & \psi_{3x} \psi_{2u}' \\ \psi_{15x} \psi_{18} & \psi_{10x} \psi_{14} & \psi_{11x} \psi_{10}' & \psi_{10x} \psi_{10}' \end{bmatrix} \quad (E-6)$$

The right half is

$$F = \begin{bmatrix} \psi_1 \psi_1' & \psi_{1x} \psi_1' + \psi_1 \psi_{1x}' & \psi_{1u} \psi_1' & \psi_1 \psi_{1u}' \\ \psi_2 \psi_2' & \psi_{2x} \psi_2' + \psi_2 \psi_{2x}' & \psi_{2u} \psi_2' & \psi_2 \psi_{2u}' \\ \psi_3 \psi_3' & \psi_{3x} \psi_3' + \psi_3 \psi_{3x}' & \psi_{3u} \psi_3' & \psi_3 \psi_{3u}' \\ \psi_2 \psi_3' & \psi_{2x} \psi_3' + \psi_2 \psi_{3x}' & \psi_{2u} \psi_3' & \psi_2 \psi_{3u}' \\ \psi_{16} \psi_{17} & \psi_{10} \psi_{13} & \psi_{12} \psi_{10}' & \psi_{10} \psi_{10}' \end{bmatrix} \quad (E-7)$$

and

$$G = \begin{bmatrix} \psi_{1x} \psi_1' & \psi_{1xx} \psi_1' + \psi_{1x} \psi_{1x}' & \psi_{1ux} \psi_1' & \psi_{1x} \psi_{1u}' \\ \psi_{2x} \psi_2' & \psi_{2xx} \psi_2' + \psi_{2x} \psi_{2x}' & \psi_{2ux} \psi_2' & \psi_{2x} \psi_{2u}' \\ \psi_{3x} \psi_3' & \psi_{3xx} \psi_3' + \psi_{3x} \psi_{3x}' & \psi_{3ux} \psi_3' & \psi_{3x} \psi_{3u}' \\ \psi_{2x} \psi_3' & \psi_{2xx} \psi_3' + \psi_{2x} \psi_{3x}' & \psi_{2ux} \psi_3' & \psi_{2x} \psi_{3u}' \end{bmatrix}$$

$$\left[ \begin{array}{cccc} \varphi_{16} \times \varphi_{17} & \varphi_{10} \times \varphi_{13} & \varphi_{12} \times \varphi_{10}' & \varphi_{10} \times \varphi_{10}' \end{array} \right] \quad (E-8)$$

where points 11, 12, 15, and 16 are local at  $(\frac{1}{3}, 0, \frac{2}{3})$ ,  $(\frac{1}{3}, \frac{2}{3}, 0)$ ,  $(0, \frac{1}{3}, \frac{2}{3})$  and  $(0, \frac{2}{3}, \frac{1}{3})$  respectively. Points 12, 13, 17 and 18 are on the non local triangle at  $(\frac{1}{3}, 0, \frac{2}{3})$ ,  $(\frac{1}{3}, \frac{2}{3}, 0)$ ,  $(0, \frac{1}{3}, \frac{2}{3})$  and  $(0, \frac{2}{3}, \frac{1}{3})$ .

Case 4 is similar. The left half is given by

$$\underline{F} = \left[ \begin{array}{cccc} \varphi_1 \varphi_1' & \varphi_{1x} \varphi_1' + \varphi_1 \varphi_{1x}' & \varphi_{1u} \varphi_1' & \varphi_1 \varphi_{1u}' \\ \varphi_3 \varphi_3' & \varphi_{3x} \varphi_3' + \varphi_3 \varphi_{3x}' & \varphi_{3u} \varphi_3' & \varphi_3 \varphi_{3u}' \\ \varphi_2 \varphi_2' & \varphi_{2x} \varphi_2' + \varphi_2 \varphi_{2x}' & \varphi_{2u} \varphi_2' & \varphi_2 \varphi_{2u}' \\ \varphi_2 \varphi_3' & \varphi_{2x} \varphi_3' + \varphi_2 \varphi_{3x}' & \varphi_{2u} \varphi_3' & \varphi_2 \varphi_{3u}' \\ \varphi_{15} \varphi_{18} & \varphi_{11} \varphi_{10}' & \varphi_{10} \varphi_{14} & \varphi_{10} \varphi_{10}' \end{array} \right] \quad (E-9)$$

$$\underline{G} = \left[ \begin{array}{cccc} \varphi_{1x} \varphi_1' & \varphi_{1xx} \varphi_1' + \varphi_{1x} \varphi_{1x}' & \varphi_{1xu} \varphi_1' & \varphi_{1x} \varphi_{1u}' \\ \varphi_{3x} \varphi_3' & \varphi_{3xx} \varphi_3' + \varphi_{3x} \varphi_{3x}' & \varphi_{3xu} \varphi_3' & \varphi_{3x} \varphi_{3u}' \\ \varphi_{2x} \varphi_2' & \varphi_{2xx} \varphi_2' + \varphi_{2x} \varphi_{2x}' & \varphi_{2xu} \varphi_2' & \varphi_{2x} \varphi_{2u}' \\ \varphi_{2x} \varphi_3' & \varphi_{2xx} \varphi_3' + \varphi_{2x} \varphi_{3x}' & \varphi_{2xu} \varphi_3' & \varphi_{2x} \varphi_{3u}' \\ \varphi_{15} \varphi_{18} & \varphi_{11x} \varphi_{10}' & \varphi_{10x} \varphi_{14} & \varphi_{10x} \varphi_{10}' \end{array} \right] \quad (E-10)$$

The right half is

$$\underline{F} = \left[ \begin{array}{cccc} \varphi_1 \varphi_1' & \varphi_{1x} \varphi_1' + \varphi_1 \varphi_{1x}' & \varphi_{1u} \varphi_1' & \varphi_1 \varphi_{1u}' \\ \varphi_2 \varphi_2' & \varphi_{2x} \varphi_2' + \varphi_2 \varphi_{2x}' & \varphi_{2u} \varphi_2' & \varphi_2 \varphi_{2u}' \\ \varphi_3 \varphi_3' & \varphi_{3x} \varphi_3' + \varphi_3 \varphi_{3x}' & \varphi_{3u} \varphi_3' & \varphi_3 \varphi_{3u}' \\ \varphi_3 \varphi_2' & \varphi_{3x} \varphi_2' + \varphi_3 \varphi_{2x}' & \varphi_{3u} \varphi_2' & \varphi_3 \varphi_{2u}' \end{array} \right]$$

$$\begin{bmatrix} \psi_{16}\psi_{17} & \psi_{12}\psi_{10}' & \psi_{10}\psi_{13} & \psi_{10}\psi_{10}' \end{bmatrix}$$

(E-11)

$$\underline{G} = \begin{bmatrix} \psi_{1x}\psi_{1'} & \psi_{1xx}\psi_{1'} + \psi_{1x}\psi_{1x}' & \psi_{1xu}\psi_{1'} & \psi_{1x}\psi_{1u}' \\ \psi_{2x}\psi_{2'} & \psi_{2xx}\psi_{2'} + \psi_{2x}\psi_{2x}' & \psi_{2xu}\psi_{2'} & \psi_{2x}\psi_{2u}' \\ \psi_{3x}\psi_{3'} & \psi_{3xx}\psi_{3'} + \psi_{3x}\psi_{3x}' & \psi_{3xu}\psi_{3'} & \psi_{3x}\psi_{3u}' \\ \psi_{3x}\psi_{2'} & \psi_{3xx}\psi_{2'} + \psi_{3x}\psi_{2x}' & \psi_{3xu}\psi_{2'} & \psi_{3x}\psi_{2u}' \\ \psi_{16x}\psi_{17} & \psi_{12x}\psi_{10}' & \psi_{10x}\psi_{13} & \psi_{10x}\psi_{10}' \end{bmatrix}$$

(E-12)

For case 4, points 11,12,15 and 16 are local at  $(\frac{1}{3}, \frac{2}{3}, 0)$

$(\frac{1}{3}, 0, \frac{2}{3})$   $(0, \frac{2}{3}, \frac{1}{3})$  and  $(0, \frac{1}{3}, \frac{2}{3})$ . Points 13,14,17 and 18 are at

$(\frac{1}{3}, \frac{2}{3}, 0)$   $(\frac{1}{3}, 0, \frac{2}{3})$ ,  $(0, \frac{2}{3}, \frac{1}{3})$  and  $(0, \frac{1}{3}, \frac{2}{3})$  on the non local

triangle.

## Appendix F - Finite Element Meshes

### 1. Streaming meshes

Mesh1

Mesh2

Mesh3

Mesh4

Mesh5

Mesh6

### 2. Scattering meshes

Mesha

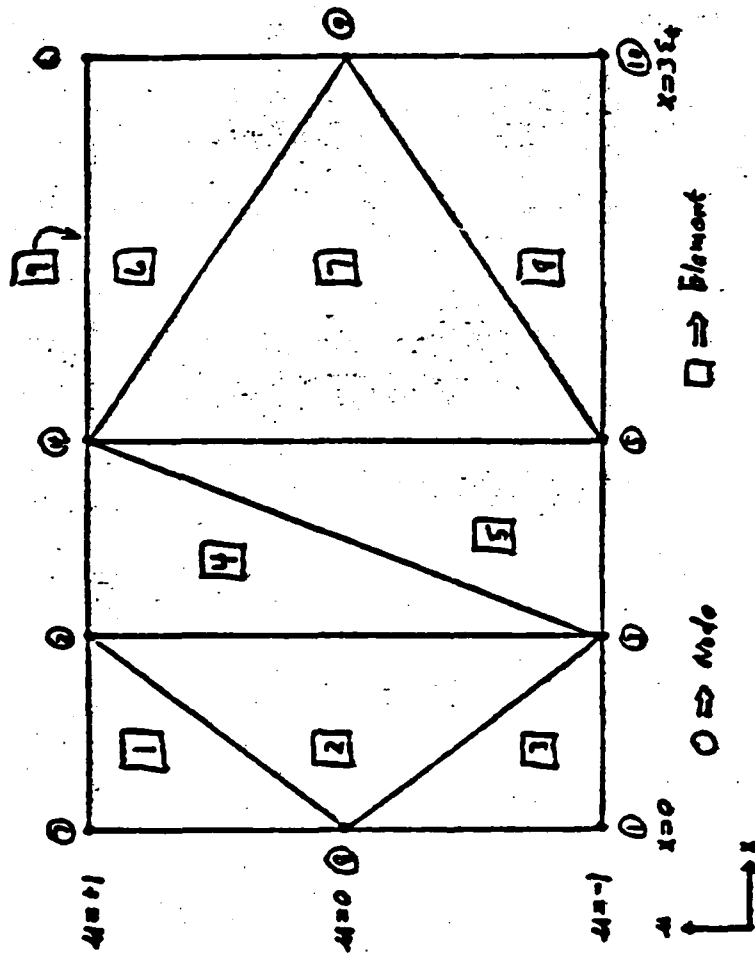
Meshb

Meshc

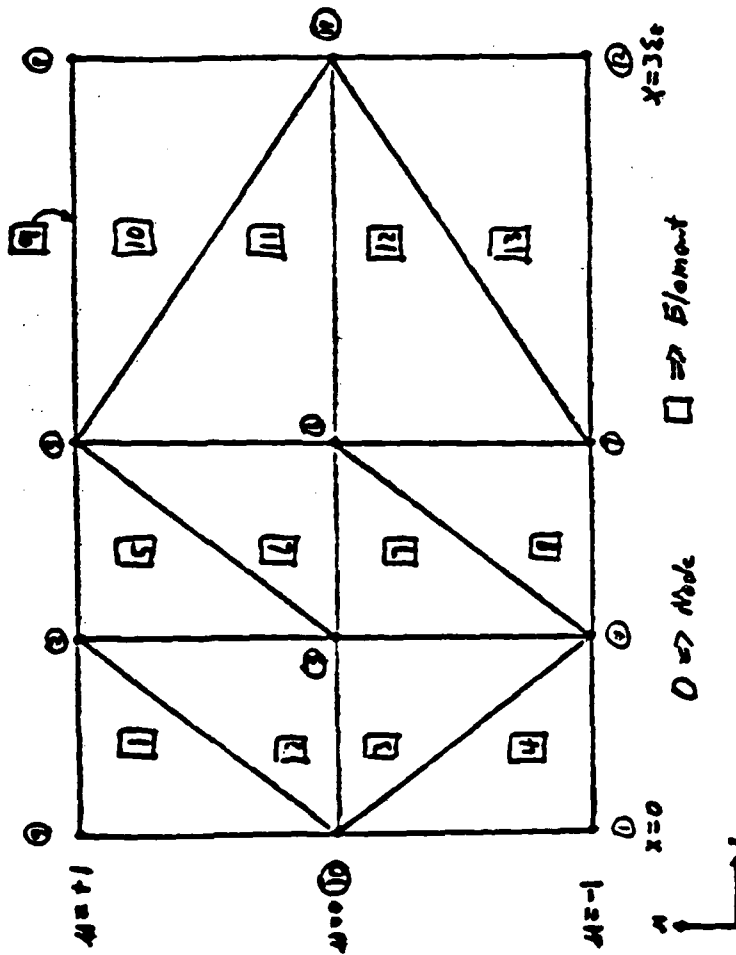
Meshd

Meshe 1 through 4 are identical to those of reference (2).

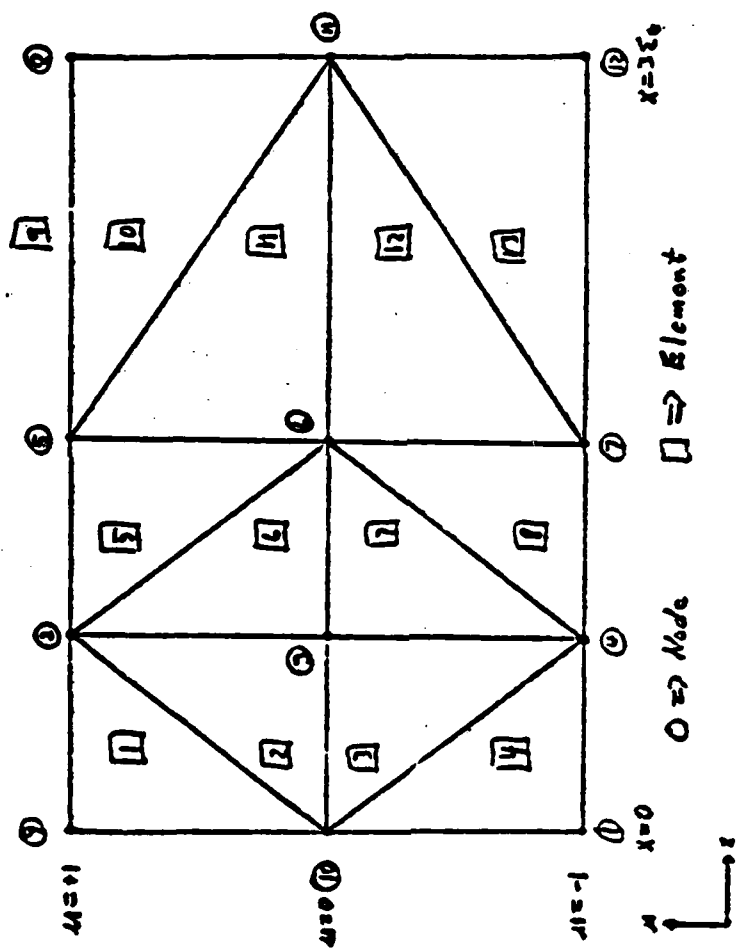
# MESH 1



# MESH 2



# MESH 3



ED MESH3

LI

1	NTRIAN	# NODE	NCOL
2	12	12	3

3	RANGE	SIGMAT	SIGMAS
4	3.	1.	.5

5	TRIANGLE	NODE1	NODE2	NODE3	COLUMN
6	1	2	9	10	1
7	2	10	3	2	1
8	3	10	4	3	1
9	4	4	10	1	1
10	5	2	6	5	2
11	6	6	2	3	2
12	7	6	3	4	2
13	8	4	7	6	2
14	9	5	11	8	3
15	10	11	5	6	3
16	11	11	6	7	3
17	12	7	12	11	3

18	COLUMN	FIRST ELEMENT	NUMBER OF ELEMENTS
19	1	1	4
20	2	5	4
21	3	9	4

22	NODE	X-AXIS	U-AXIS
23	1	.000	-1.000
24	2	.250	1.000
25	3	.250	.000
26	4	.250	-1.000
27	5	.500	1.000
28	6	.500	.000
29	7	.500	-1.000
30	8	1.000	1.000
31	9	.000	1.000
32	10	.000	.000
33	11	1.000	.000
34	12	1.000	-1.000

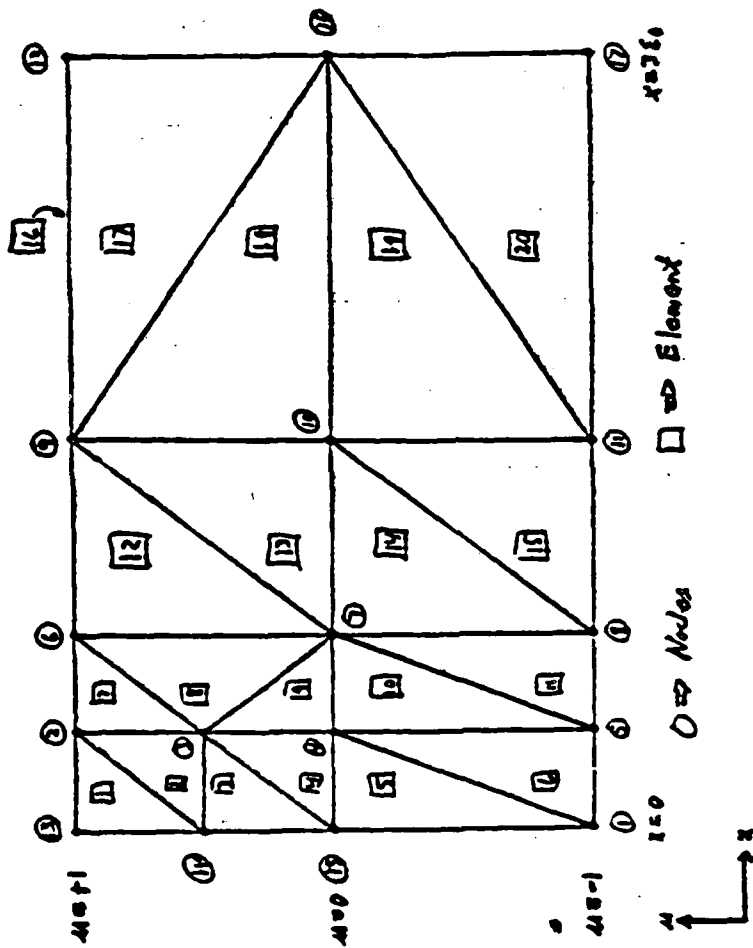
39

EOF..

EOT..

UP

**MESH 4**



**F--B**

ED MSHC3.5C

LI,1,200

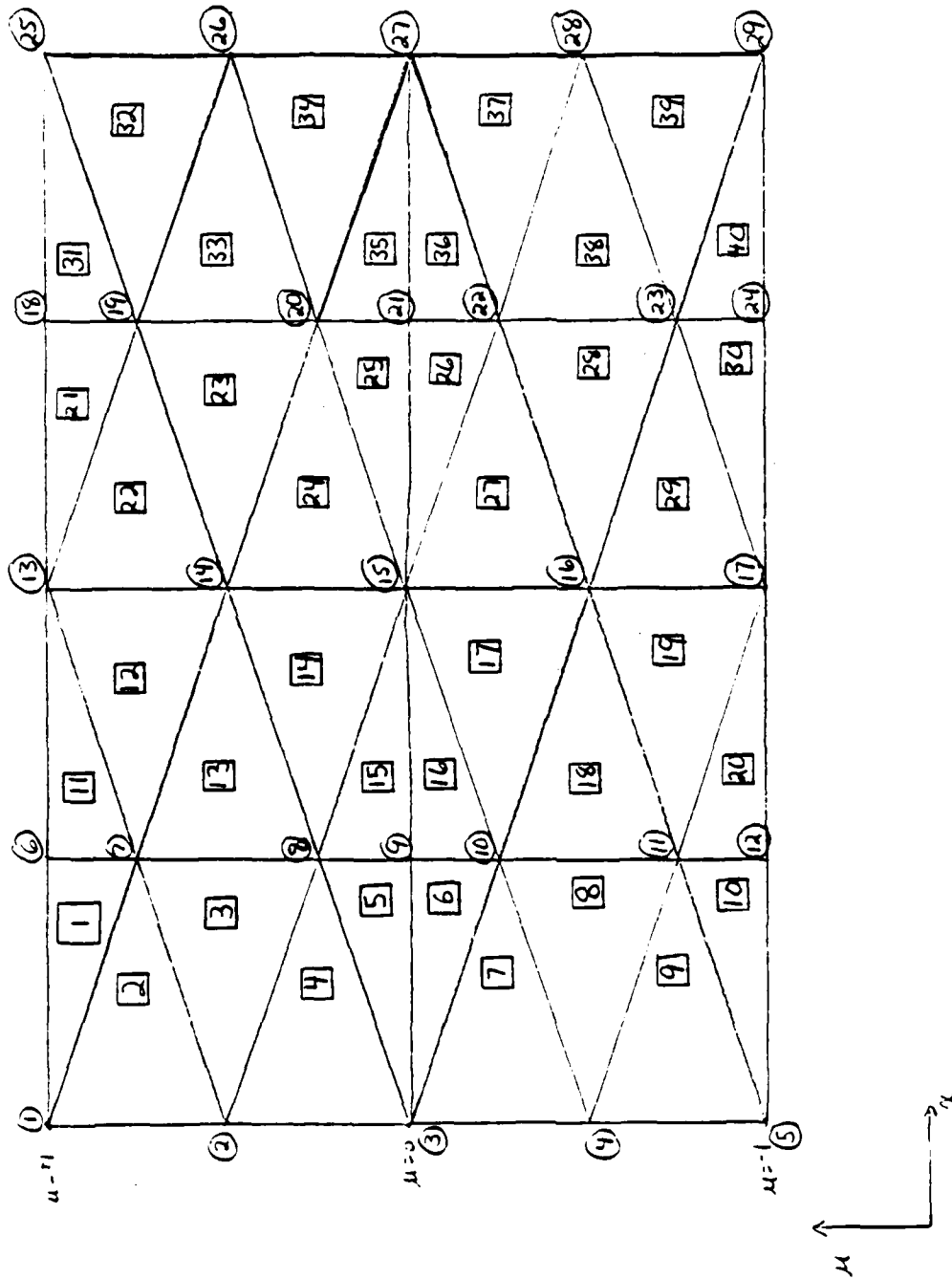
1	NTRIAN	MNODE	NCOL
2	40	29	4

4	RANGE	SIGMAT	SIGMAS
5	3.	1.	.5

7	TRIANGLE	NODE1	NODE2	NODE3	COLUMN
8	1	1	7	6	1
9	2	7	1	2	1
10	3	2	8	7	1
11	4	8	2	3	1
12	5	3	9	8	1
13	6	3	10	9	1
14	7	10	3	4	1
15	8	4	11	10	1
16	9	11	4	5	1
17	10	5	12	11	1
18	11	13	6	7	2
19	12	7	14	13	2
20	13	14	7	8	2
21	14	8	15	14	2
22	15	15	8	9	2
23	16	15	9	10	2
24	17	10	16	15	2
25	18	16	10	11	2
26	19	11	17	16	2
27	20	17	11	12	2
28	21	13	19	18	3
29	22	19	13	14	3
30	23	14	20	19	3
31	24	20	14	15	3
32	25	15	21	20	3
33	26	15	22	21	3
34	27	22	15	16	3
35	28	16	23	22	3
36	29	23	16	17	3
37	30	17	24	23	3
38	31	25	18	19	4
39	32	19	26	25	4
40	33	26	19	20	4
41	34	20	27	26	4
42	35	27	20	21	4
43	36	27	21	22	4
44	37	22	28	27	4
45	38	28	22	23	4
46	39	23	29	28	4
47	40	29	23	24	4

49	COLUMN	FIRST ELEMENT	NUMBER OF ELEMENTS
50	1	1	10
51	2	11	10
52	3	21	10
53	4	31	10
54			

# FIG. C



ED MSHB3.9C

LI,1,100

1	NTRIAN	MNODE	NCOL
2	12	11	2

3	RANGE	SIGMAT	SIGMAS
4	3.	1.	.9

6	TRIANGLE	NODE1	NODE2	NODE3	COLUMN
7	1	1	5	4	1
8	2	5	1	2	1
9	3	2	6	5	1
10	4	2	7	6	1
11	5	7	2	3	1
12	6	3	8	7	1
13	7	9	4	5	2
14	8	5	10	9	2
15	9	10	5	6	2
16	10	10	6	7	2
17	11	7	11	10	2
18	12	11	7	8	2

20	COLUMN	FIRST ELEMENT	NUMBER OF ELEMENTS
21	1	1	6
22	2	7	6

24	NODE	X-AXIS	U-AXIS
25	1	.000	1.000
26	2	.000	.000
27	3	.000	-1.000
28	4	.500	1.000
29	5	.500	.500
30	6	.500	.000
31	7	.500	-.500
32	8	.500	-1.000
33	9	1.000	1.000
34	10	1.000	.000
35	11	1.000	-1.000

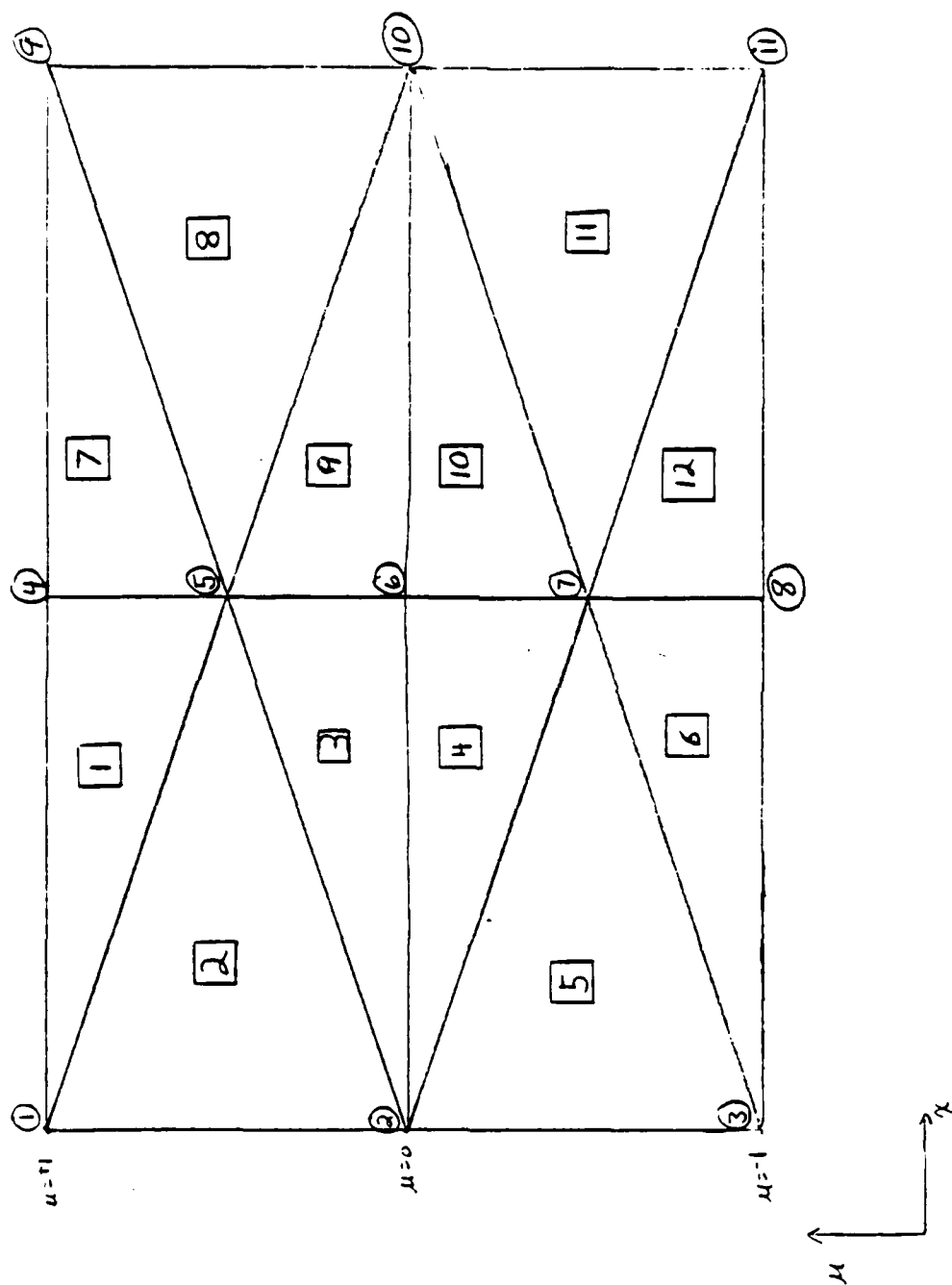
37	NODE (NB)	FLUX
38	8	
39	1	3.5345E-01
40	3	4.0360E-02
41	4	2.5000E-01
42	6	2.1768E-01
43	28	4.2659E-02
44	30	1.9896E-02
45	31	2.7962E-02
46	33	1.0452E-02

EOF..

EOT..

UP

# MESH B



ED MSHA3.5C

LI

1	NTRIAN	MNODE	NCOL
2	4	6	1

3

4	RANGE	SIGMAT	SIGMAS
5	3.	1.	.5

6

7	TRIANGLE	NODE1	NODE2	NODE3	COLUMN
8	1	4	1	2	1
9	2	2	5	4	1
10	3	5	2	3	1
11	4	3	6	5	1

12

13	COLUMN	FIRST ELEMENT	NUMBER OF ELEMENTS
14	1	1	4

15

16	NODE	X-AXIS	U-AXIS
17	1	.000	1.000
18	2	.000	.000
19	3	.000	-1.000
20	4	1.000	1.000
21	5	1.000	.000
22	6	1.000	-1.000

23

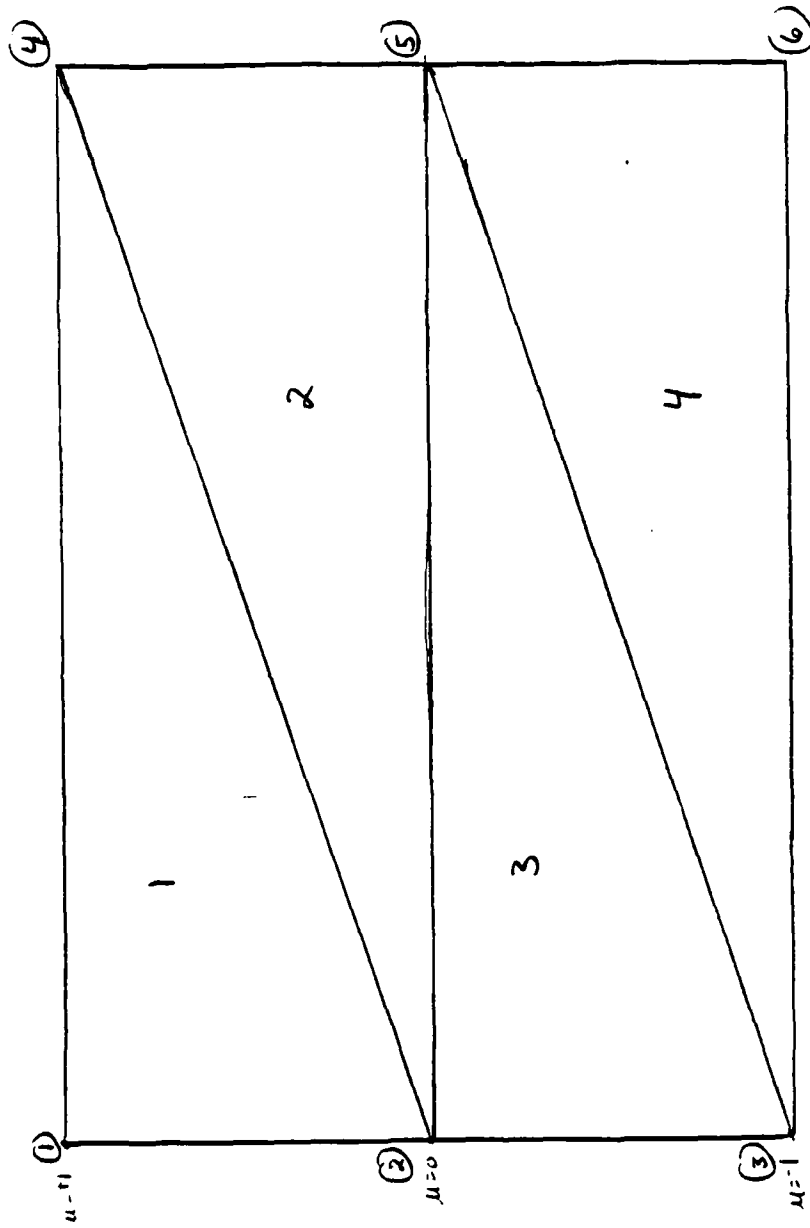
24	NODE (NB)	FLUX
25	8	
26	1	1.0142E+00
27	3	9.8832E-01
28	4	1.2126E-01
29	6	6.1684E-01
30	13	6.5917E-03
31	15	5.3892E-03
32	16	3.2862E-03
33	18	1.9460E-03

EOF..

EOT..

UP

MESH A



111	12	.250	.000
112	13	.250	-1.000
113	14	.375	1.000
114	15	.375	.750
115	16	.375	.500
116	17	.375	.250
117	18	.375	.000
118	19	.375	-1.000
119	20	.500	1.000
120	21	.500	.750
121	22	.500	.500
122	23	.500	.250
123	24	.500	.000
124	25	.500	-1.000
125	26	.625	1.000
126	27	.625	.750
127	28	.625	.500
128	29	.625	.250
129	30	.625	.000
130	31	.625	-1.000
131	32	.750	1.000
132	33	.750	.750
133	34	.750	.500
134	35	.750	.250
135	36	.750	.000
136	37	.750	-1.000
137	38	.875	1.000
138	39	.875	.750
139	40	.875	.500
140	41	.875	.250
141	42	.875	.000
142	43	.875	-1.000
143	44	1.000	1.000
144	45	1.000	.750
145	46	1.000	.500
146	47	1.000	.250
147	48	1.000	.000
148	49	1.000	-1.000
149	50	.000	1.000
150	51	.000	.750
151	52	.000	.500
152	53	.000	.250
153	54	.000	.000
154			
EOF..			
EOT..			

55	48	24	30	29	5
56	49	30	24	25	5
57	50	25	31	30	5
58	51	32	26	27	6
59	52	27	33	32	6
60	53	33	27	28	6
61	54	28	34	33	6
62	55	34	28	29	6
63	56	29	35	34	6
64	57	35	29	30	6
65	58	30	36	35	6
66	59	36	30	31	6
67	60	31	37	36	6
68	61	38	32	33	7
69	62	33	39	38	7
70	63	39	33	34	7
71	64	34	40	39	7
72	65	40	34	35	7
73	66	35	41	40	7
74	67	41	35	36	7
75	68	36	42	41	7
76	69	42	36	37	7
77	70	37	43	42	7
78	71	44	38	39	8
79	72	39	45	44	8
80	73	45	39	40	8
81	74	40	46	45	8
82	75	46	40	41	8
83	76	41	47	46	8
84	77	47	41	42	8
85	78	42	48	47	8
86	79	48	42	43	8
87	80	43	49	48	8

	COLUMN	FIRST ELEMENT	NUMBER OF ELEMENTS
88			
89	1	1	10
90	2	11	10
91	3	21	10
92	4	31	10
93	5	41	10
94	6	51	10
95	7	61	10
96	8	71	10
97			
98			
	NODE	X-AXIS	U-AXIS
99			
100	1	.000	-1.000
101	2	.125	1.000
102	3	.125	.750
103	4	.125	.500
104	5	.125	.250
105	6	.125	.000
106	7	.125	-1.000
107	8	.250	1.000
108	9	.250	.750
109	10	.250	.500
110	11	.250	.250

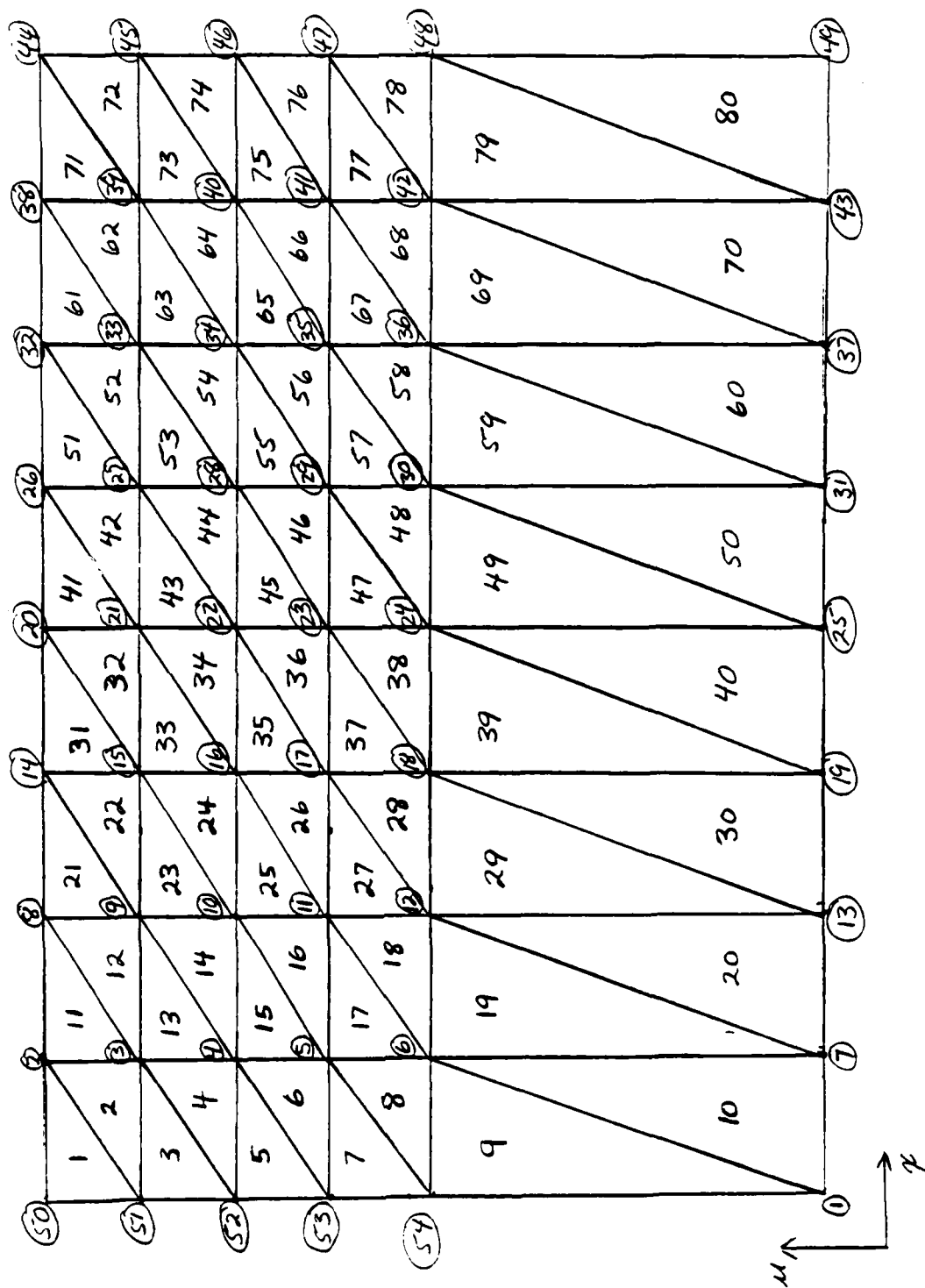
ED MESH6

LI,1,200

1	NTRIAN	# NODE	NCOL
2	80	54	8
4	RANGE	SIGMAT	SIGMAS
5	3.	1.	.5

7	TRIANGLE	NODE1	NODE2	NODE3	COLUMN
8	1	2	50	51	1
9	2	51	3	2	1
10	3	3	51	52	1
11	4	52	4	3	1
12	5	4	52	53	1
13	6	53	5	4	1
14	7	5	53	54	1
15	8	54	6	5	1
16	9	6	54	1	1
17	10	1	7	6	1
18	11	8	2	3	2
19	12	3	9	8	2
20	13	9	3	4	2
21	14	4	10	9	2
22	15	10	4	5	2
23	16	5	11	10	2
24	17	11	5	6	2
25	18	6	12	11	2
26	19	12	6	7	2
27	20	7	13	12	2
28	21	14	8	9	3
29	22	9	15	14	3
30	23	15	9	10	3
31	24	10	16	15	3
32	25	16	10	11	3
33	26	11	17	16	3
34	27	17	11	12	3
35	28	12	18	17	3
36	29	18	12	13	3
37	30	13	19	18	3
38	31	20	14	15	4
39	32	15	21	20	4
40	33	21	15	16	4
41	34	16	22	21	4
42	35	22	16	17	4
43	36	17	23	22	4
44	37	23	17	18	4
45	38	18	24	23	4
46	39	24	18	19	4
47	40	19	25	24	4
48	41	26	20	21	5
49	42	21	27	26	5
50	43	27	21	22	5
51	44	22	28	27	5
52	45	28	22	23	5
53	46	23	29	28	5
54	47	29	23	24	5

# TEST 6



55	9	.250	.750
56	10	.250	.500
57	11	.250	.250
58	12	.250	-1.000
59	13	.500	1.000
60	14	.500	.750
61	15	.500	.500
62	16	.500	-1.000
63	17	1.000	1.000
64	18	1.000	.750
65	19	1.000	-1.000
66	20	.000	1.000
67	21	.000	.750
68	22	.000	.500
69	23	.000	.250
70	24	.000	.000
71			
EOF..			
EOT..			
UP			

## ED MESH5

LI

1	NTRIAN	# NODE	NCOL		
2	31	24	4		
3					
4	RANGE	SIGMAT	SIGMAS		
5	3.	1.	.5		
6					
7	TRIANGLE	NODE1	NODE2	NODE3	COLUMN
8	1	2	20	21	1
9	2	21	3	2	1
10	3	3	21	22	1
11	4	22	4	3	1
12	5	4	22	23	1
13	6	23	5	4	1
14	7	5	23	24	1
15	8	24	6	5	1
16	9	6	24	1	1
17	10	1	7	6	1
18	11	8	2	3	2
19	12	3	9	8	2
20	13	9	3	4	2
21	14	4	10	9	2
22	15	10	4	5	2
23	16	5	11	10	2
24	17	11	5	6	2
25	18	6	12	11	2
26	19	12	6	7	2
27	20	13	8	9	3
28	21	9	14	13	3
29	22	14	9	10	3
30	23	10	15	14	3
31	24	15	10	11	3
32	25	11	16	15	3
33	26	16	11	12	3
34	27	17	13	14	4
35	28	14	18	17	4
36	29	18	14	15	4
37	30	15	19	18	4
38	31	19	15	16	4
39					
40	COLUMN	FIRST ELEMENT	NUMBER OF	ELEMENTS	
41	1	1	10		
42	2	11	9		
43	3	20	7		
44	4	27	5		
45					
46	NODE	X-AXIS	U-AXIS		
47	1	.000	-1.000		
48	2	.125	1.000		
49	3	.125	.750		
50	4	.125	.500		
51	5	.125	.250		
52	6	.125	.000		
53	7	.125	-1.000		
54	8	.250	1.000		

ED MESH4

LI

	NTRIAN	* NODE	NCOL
1			
2	19	17	4
3			
4	RANGE	SIGMAT	SIGMAS
5	3.	1.	.5

	TRIANGLE	NODE1	NODE2	NODE3	COLUMN
8	1	2	13	14	1
9	2	14	3	2	1
10	3	3	14	15	1
11	4	15	4	3	1
12	5	4	15	1	1
13	6	1	5	4	1
14	7	6	2	3	2
15	8	3	7	6	2
16	9	7	3	4	2
17	10	7	4	5	2
18	11	5	8	7	2
19	12	9	6	7	3
20	13	7	10	9	3
21	14	10	7	8	3
22	15	8	11	10	3
23	16	9	16	12	4
24	17	16	9	10	4
25	18	16	10	11	4
26	19	11	17	16	4

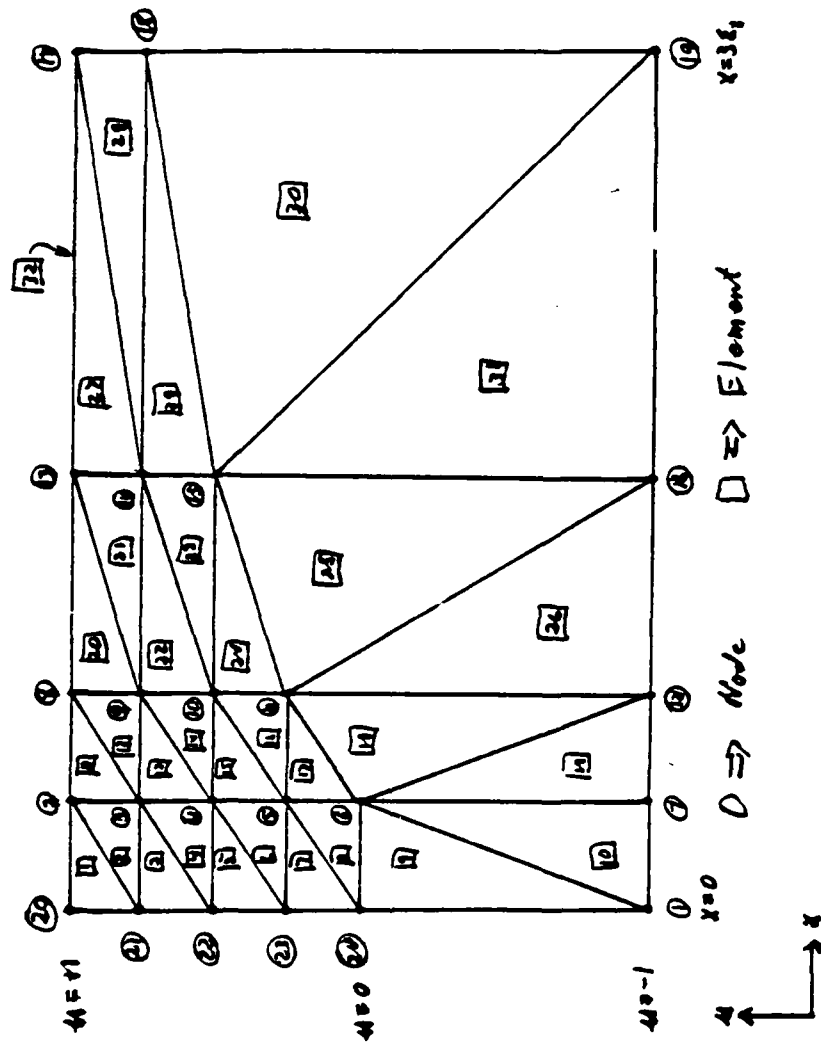
	COLUMN	FIRST ELEMENT	NUMBER OF ELEMENTS
27			
28			
29	1	1	6
30	2	7	5
31	3	12	4
32	4	16	4

	NODE	X-AXIS	U-AXIS
33			
34			
35	1	.000	-1.000
36	2	.125	1.000
37	3	.125	.500
38	4	.125	.000
39	5	.125	-1.000
40	6	.250	1.000
41	7	.250	.000
42	8	.250	-1.000
43	9	.500	1.000
44	10	.500	.000
45	11	.500	-1.000
46	12	1.000	1.000
47	13	.000	1.000
48	14	.000	.500
49	15	.000	.000
50	16	1.000	.000
51	17	1.000	-1.000

EOF..

EOT..

# MESH 5



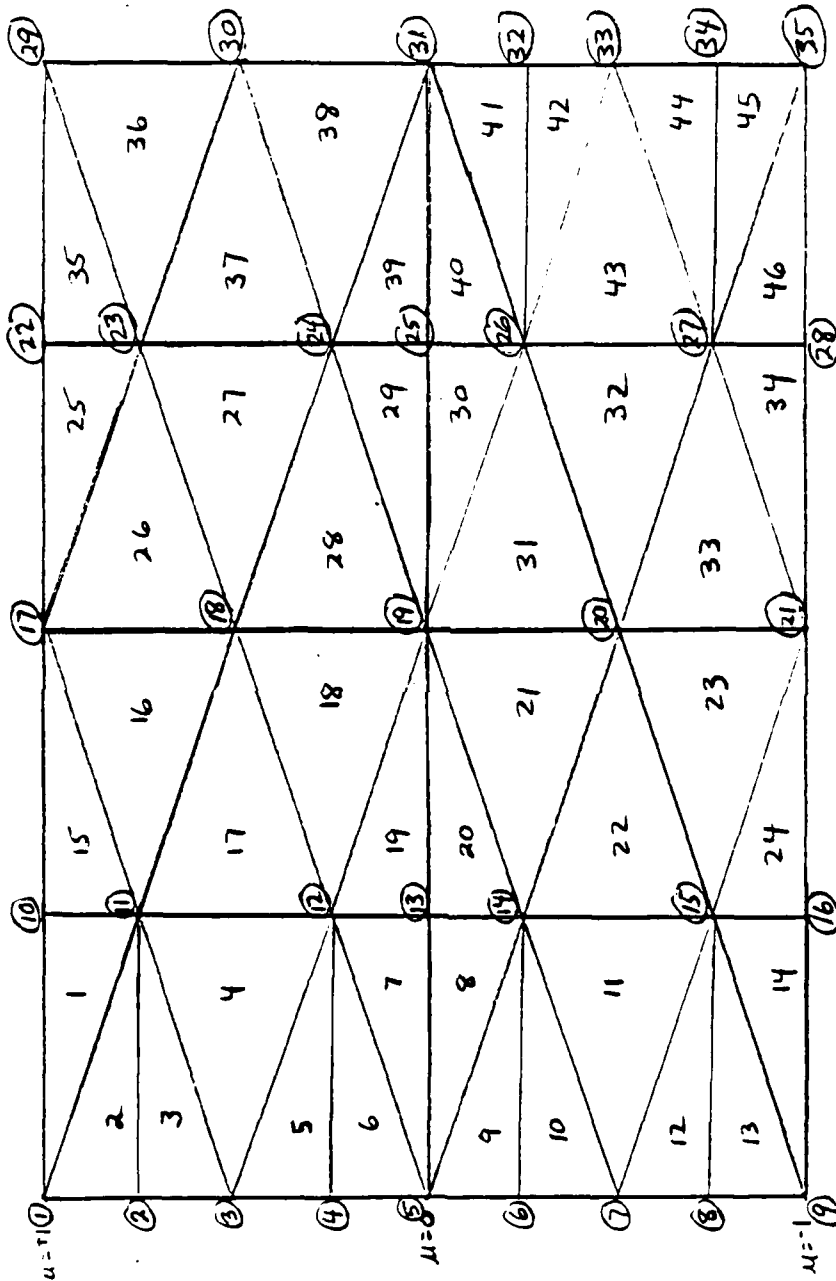
1

	NODE	X-AXIS	U-AXIS
55			
56	1	0.000	1.000
57	2	0.000	0.500
58	3	0.000	0.000
59	4	0.000	-0.500
60	5	0.000	-1.000
61	6	0.250	1.000
62	7	0.250	0.750
63	8	0.250	0.250
64	9	0.250	0.000
65	10	0.250	-0.250
66	11	0.250	-0.750
67	12	0.250	-1.000
68	13	0.500	1.000
69	14	0.500	0.500
70	15	0.500	0.000
71	16	0.500	-0.500
72	17	0.500	-1.000
73	18	0.750	1.000
74	19	0.750	0.750
75	20	0.750	0.250
76	21	0.750	0.000
77	22	0.750	-0.250
78	23	0.750	-0.750
79	24	0.750	-1.000
80	25	1.000	1.000
81	26	1.000	0.500
82	27	1.000	0.000
83	28	1.000	-0.500
84	29	1.000	-1.000

	NODE (NB)	FLUX
85		
86	12	
87	1	1.0142E+00
88	3	9.8832E-01
89	4	5.2627E-01
90	6	9.8330E-01
91	7	1.2126E-01
92	9	6.1684E-01
93	79	6.5917E-03
94	81	5.3892E-03
95	82	4.4268E-03
96	84	2.9434E-03
97	85	3.2862E-03
98	87	1.9460E-03
99		

EDT..  
UP

TEST D



ED MSHD3.5C

LI,1,200

1	NTRIAN	MNODE	NCOL		
2	46	35	4		
3					
4	RANGE	SIGMAT	SIGMAS		
5	3.	1.	.5		
6					
7	TRIANGLE	NODE1	NODE2	NODE3	COLUMN
8	1	1	11	10	1
9	2	11	1	2	1
10	3	11	2	3	1
11	4	3	12	11	1
12	5	12	3	4	1
13	6	12	4	5	1
14	7	5	13	12	1
15	8	5	14	13	1
16	9	14	5	6	1
17	10	14	6	7	1
18	11	7	15	14	1
19	12	15	7	8	1
20	13	15	8	9	1
21	14	9	16	15	1
22	15	17	10	11	2
23	16	11	18	17	2
24	17	18	11	12	2
25	18	12	19	18	2
26	19	19	12	13	2
27	20	19	13	14	2
28	21	14	20	19	2
29	22	20	14	15	2
30	23	15	21	20	2
31	24	21	15	16	2
32	25	17	23	22	3
33	26	23	17	18	3
34	27	18	24	23	3
35	28	24	18	19	3
36	29	19	25	24	3
37	30	19	26	25	3
38	31	26	19	20	3
39	32	20	27	26	3
40	33	27	20	21	3
41	34	21	28	27	3
42	35	29	22	23	4
43	36	23	30	29	4
44	37	30	23	24	4
45	38	24	31	30	4
46	39	31	24	25	4
47	40	31	25	26	4
48	41	26	32	31	4
49	42	26	33	32	4
50	43	33	26	27	4
51	44	27	34	33	4
52	45	27	35	34	4
53	46	35	27	28	4
54					

	COLUMN	FIRST ELEMENT	NUMBER OF ELEMENTS
55	1	1	14
56	2	15	10
57	3	25	10
58	4	35	12

	NODE	X-AXIS	U-AXIS
61	1	0.000	1.000
62	2	0.000	0.750
63	3	0.000	0.500
64	4	0.000	0.250
65	5	0.000	0.000
66	6	0.000	-0.250
67	7	0.000	-0.500
68	8	0.000	-0.750
69	9	0.000	-1.000
70	10	0.250	1.000
71	11	0.250	0.750
72	12	0.250	0.250
73	13	0.250	0.000
74	14	0.250	-0.250
75	15	0.250	-0.750
76	16	0.250	-1.000
77	17	0.500	1.000
78	18	0.500	0.500
79	19	0.500	0.000
80	20	0.500	-0.500
81	21	0.500	-1.000
82	22	0.750	1.000
83	23	0.750	0.750
84	24	0.750	0.250
85	25	0.750	0.000
86	26	0.750	-0.250
87	27	0.750	-0.750
88	28	0.750	-1.000
89	29	1.000	1.000
90	30	1.000	0.500
91	31	1.000	0.000
92	32	1.000	-0.250
93	33	1.000	-0.500
94	34	1.000	-0.750
95	35	1.000	-1.000

	NODE (NB)	FLUX
96	20	
97	1	1.0142E+00
98	3	9.8832E-01
99	4	7.6712E-01
100	6	9.7586E-01
101	7	5.2627E-01
102	9	9.8330E-01
103	10	2.7547E-01
104	12	8.1002E-01
105	13	1.2126E-01
106	15	6.1684E-01
107	91	6.5917E-03

111	93	5.3892E-03
112	94	5.2444E-03
113	96	4.3298E-03
114	97	4.4268E-03
115	99	2.9434E-03
116	100	3.7727E-03
117	102	2.2812E-03
118	103	3.2862E-03
119	105	1.9460E-03

EOT..

Appendix G - Subroutines to numerically evaluate the scattering  
integral

Glossary of Variables

x1,x2,x3,u1,u2,u3 - triangle geometric coordinates

x(49),u(49) - coordinates of 49 integration points

MC - coefficient matrix of eqn 2-4

DET - deteminate of MC

DU(7) - delta u at each of the seven

spatial integration points

LX(3) - derivatives of  $l_1, l_2$  and  $l_3$  w.r.t.  $\gamma$

DX(mntria) - column width

L (49,3) - array storing natural coordinates of integration  
points

M(49,10) - array storing m of 2-29 evaluated at the integration  
points

MX(49,10) - array of  $m_x$  of 2-30

NLM - non local matrix

LI - local integral sum of  $\int u \frac{\partial \phi}{\partial x} du + \int \phi du$

NLI - non local integral  $\int \phi' du'$

ILDF - integral local derivative of flux

FLUX(49,10) - flux at integration points

DFLUX(49,10) - derivative of flux

UI1,UI2,...,UI7 - u integrals at the seven points needed for  
spatial integration

```

LI,1,160
1 *****
2
3
4     SUBROUTINE LCORD(AREAS,TRI,PTNODE,CORDND,M,MX,DU,DX,U,X)
5
6     PARAMETER (MNODE=151 , MNTRIA=46)
7     DOUBLE PRECISION X1,X2,X3,U1,U2,U3,XX(7),X(49),U(49)
8     DOUBLE PRECISION MC(3,3),DET,DU(7),LX(3),DX(MNTRIA),L(49,3)
9     DOUBLE PRECISION AREAS(MNTRIA),CORDND(MNODE,2),M(49,10),MX(49,
10    DOUBLE PRECISION ML(MNTRIA,10,10),MG(MNODE,MNODE)
11    DOUBLE PRECISION NLM(MNTRIA,14,10,10),LI(MNTRIA,10,7)
12    DOUBLE PRECISION NLI(MNTRIA,7,10),AS(MNODE*(MNODE-1)/2),F,G
13    INTEGER CASE,TRI,PTNODE(MNTRIA,11)
14    COMMON MG,ML,NLM,LI,NLI,AS
15
16 * THIS SUBROUTINE FINDS THE NATURAL COORDINATES NEEDED FOR
17 * NUMERICAL INTEGRATION OF THE SCATTERING INTEGRAL
18 * 49 POINTS FOR WEDDLES N=6
19
20 * GET THE (X,U) COORDINATES OF THE TRIANGLE
21    X1=CORDND(PTNODE(TRI,1),1)
22    X2=CORDND(PTNODE(TRI,4),1)
23    X3=CORDND(PTNODE(TRI,7),1)
24    U1=CORDND(PTNODE(TRI,1),2)
25    U2=CORDND(PTNODE(TRI,4),2)
26    U3=CORDND(PTNODE(TRI,7),2)
27
28 * DETERMINE THE ORIENTATION OF THE ELEMENT
29    CASE=2
30    IF (X1.GT.X2) THEN
31        CASE=1
32    ENDIF
33
34 * GET X COORDS OF NUMERICAL INTEGRATION POINTS
35    XX(1)=MIN(X1,X2,X3)
36    XX(7)=MAX(X1,X2,X3)
37    F=(XX(7)-XX(1))/6.0
38    DO 50 I=2,6
39        XX(I)=XX(1)+(I-1)*F
40 50    CONTINUE
41    DO 70 I=1,7
42        J=7*I-6
43        DO 60 K=J,J+6
44            X(K)=XX(I)
45 60    CONTINUE
46 70    CONTINUE
47
48
49 * GET U COORDS OF THE SAME POINTS
50    IF (CASE.EQ.1) THEN
51        U(1)=U3
52        U(7)=U2
53        F=(U1-U3)/6.0
54        G=(U1-U2)/6.0
55    DO 80 I=8,36,7

```

```

56         J=(I-1)/7
57         U(I)=U3+J*F
58         U(I+6)=U2+J*G
59 80      CONTINUE
60         U(43)=U1
61         U(49)=U1
62      ELSE
63         U(1)=U1
64         U(7)=U1
65         F=(U2-U1)/6.0
66         G=(U3-U1)/6.0
67         DO 95 I=8,36,7
68             J=(I-1)/7
69             U(I)=U1+J*F
70             U(I+6)=U1+J*G
71 95      CONTINUE
72         U(43)=U2
73         U(49)=U3
74      ENDIF
75      DO 100 I=1,43,7
76          F=(U(I+6)-U(I))/6.0
77          DO 98 J=1,5
78              U(I+J)=U(I)+J*F
79 98      CONTINUE
80 100     CONTINUE
81
82 * COMPUTE THE LOCAL NATURAL COORDINATES
83 * INVERSE USING ADJOINT AND DETERMINANT
84      DET=2.0*AREAS(TRI)
85      MC(1,1)=(X2*U3-X3*U2)/DET
86      MC(1,2)=(U2-U3)/DET
87      MC(1,10)=(X3-X2)/DET
88      MC(2,1)=(X3*U1-X1*U3)/DET
89      MC(2,2)=(U3-U1)/DET
90      MC(2,3)=(X1-X3)/DET
91      MC(3,1)=(X1*U2-X2*U1)/DET
92      MC(3,2)=(U1-U2)/DET
93      MC(3,3)=(X2-X1)/DET
94
95 * ASSEMBLE THE NATURAL COORDINATES INTO ARRAY L(49,3)
96      DO 110 I=1,49
97          DO 105 J=1,3
98              L(I,J)=MC(J,1) + MC(J,2)*X(I) + MC(J,3)*U(I)
99 105      CONTINUE
100 110     CONTINUE
101
102 * FIND DELTA U AT THE SEVEN LOCATIONS WHERE INTEGRATION
103 * OVER U IS NECESSARY
104      DO 120 I=1,7
105          J=(I-1)*7+1
106          DU(I)=U(J+6)-U(J)
107 120     CONTINUE
108
109 * ASSEMBLE DERIVATIVES OF NATURAL COORDINATES INTO LX(3)
110 * AND CALCULATE INTERVAL WIDTH FOR X INTEGRATION
111      LX(1)=(U2-U3)/DET

```

```

112      LX(2)=(U3-U1)/DET
113      LX(3)=(U1-U2)/DET
114      DX(TRI)=X(49)-X(1)
115
116 * EVALUATE M AND dM/dX AT THE 49 INTEGRATION POINTS
117      DO 150 I=1,49
118          M(I,1)=L(I,1)**3
119          MX(I,1)=3.0*(L(I,1)**2)*LX(1)
120          M(I,2)=L(I,1)**2 * L(I,2)
121          MX(I,2)=L(I,1)*L(I,2)*2.0*LX(1) + L(I,1)**2 * LX(2)
122          M(I,3)=L(I,1)**2 * L(I,3)
123          MX(I,3)=L(I,1)*L(I,3)*2.0*LX(1) + L(I,1)**2 * LX(3)
124          M(I,4)=L(I,2)**3
125          MX(I,4)=L(I,2)**2 *3.0*LX(2)
126          M(I,5)=L(I,2)**2 *L(I,3)
127          MX(I,5)=L(I,2)*2.0*L(I,3)*LX(2) + L(I,2)**2 *LX(3)
128          M(I,6)=L(I,2)**2 *L(I,1)
129          MX(I,6)=L(I,2)*2.0*LX(2)*L(I,1) + L(I,2)**2 *LX(1)
130          M(I,7)=L(I,3)**3
131          MX(I,7)=3.0*L(I,3)**2 * LX(3)
132          M(I,8)=L(I,3)**2 *L(I,1)
133          MX(I,8)=2.0*LX(3)*L(I,3)*L(I,1) + L(I,3)**2 *LX(1)
134          M(I,9)=L(I,3)**2 *L(I,2)
135          MX(I,9)=2.0*L(I,3)*LX(3)*L(I,2) + L(I,3)**2 *LX(2)
136          M(I,10)=L(I,1)*L(I,2)*L(I,3)
137          MX(I,10)=LX(1)*L(I,2)*L(I,3) +LX(2)*L(I,1)*L(I,3)
138          MX(I,10)=MX(I,10) + LX(3)*L(I,1)*L(I,2)
139 150      CONTINUE
140      END
141
EOF..
EOT..

```

```

LI,1,100
1 *****
2
3 * THIS SUBROUTINE PERFORMS WEDDLES N=6 RULE INTEGRATION OVER
4 * A TRIANGLE, IN THE U DIRECTION, AT THE SEVEN
5 * X COORDINATES, FOR USE IN THE NUMERICAL INTEGRATION OVER
6 * SPACE IN SUBROUTINE ISPACE
7
8     SUBROUTINE ANING(DU,M,GT,MX,U,TRI,SIGMAT,SIGMAS,X,CORDND)
9
10     PARAMETER (MNODE=151 , MNTRIA=46)
11     DOUBLE PRECISION DU(7),M(49,10),GT(10,10),ILDF(10,10)
12     DOUBLE PRECISION U(49),MX(49,10),DFLUX(49,10),FLUX(49,10)
13     DOUBLE PRECISION ML(MNTRIA,10,10),MG(MNODE,MNODE)
14     DOUBLE PRECISION NLM(MNTRIA,14,10,10),LI(MNTRIA,10,7)
15     DOUBLE PRECISION NLI(MNTRIA,7,10),AS(MNODE*(MNODE-1)/2)
16     DOUBLE PRECISION SIGMAT,SIGMAS,A,B
17     DOUBLE PRECISION X(49),CORDND(MNODE,2)
18     INTEGER TRI
19     COMMON MG,ML,NLM,LI,NLI,AS
20
21 * CALCULATE FLUX AT THE FORTY NINE INTEGRATION POINTS
22 * AND CALCULATE THE DERIVATIVE OF FLUX IN THE X DIRECTION
23 * AT THE INTEGRATION POINTS
24     DO 100 I=1,49
25         DO 50 J=1,10
26             FLUX(I,J)=0.0
27             DFLUX(I,J)=0.0
28             DO 25 K=1,10
29                 FLUX(I,J)=FLUX(I,J) + M(I,K)*GT(K,J)
30                 DFLUX(I,J)=DFLUX(I,J) + MX(I,K)*GT(K,J)
31 25     CONTINUE
32 50     CONTINUE
33 100    CONTINUE
34
35 * CALCULATE THE INTEGRAL OF FLUX OVER U
36 * AT THE SEVEN SPATIAL INTEGRAL POINTS
37 * PLACE IN ROWS, THIS IS NON-LOCAL INTEGRAL
38     DO 200 I=1,7
39         K=7*I-6
40         DO 150 J=1,10
41             NLI(TRI,I,J)=(DU(I)/20.0)*(FLUX(K,J)+5.0*FLUX(K+1,J)
42             C +FLUX(K+2,J)+6.0*FLUX(K+3,J)+FLUX(K+4,J)+5.0*FLUX(K+5,J)
43             C +FLUX(K+6,J))
44 150    CONTINUE
45 200    CONTINUE
46
47
48 * CALCULATE INTEGRAL U*DFLUX - ARANGE INTO COLUMNS, ADD
49 * NLI TO OBTAIN THE LOCAL INTEGRAL
50     A=-SIGMAS
51     B=.5*SIGMAS*SIGMAS - SIGMAS*SIGMAT
52
53     DO 300 I=1,7
54         K=7*I-6
55         DO 250 J=1,10

```

```

56             ILDF(I,J)=(DU(I)/20.0)*(DFLUX(K,J)*U(K)+5.0*DFLUX(K+1,
57 C *U(K+1)+DFLUX(K+2,J)*U(K+2)+6.0*DFLUX(K+3,J)*U(K+3)+
58 C DFLUX(K+4,J)*U(K+4)+5.0*DFLUX(K+5,J)*U(K+5)+
59 C DFLUX(K+6,J)*U(K+6))*A
60 250         CONTINUE
61 300         CONTINUE
62         DO 400 I=1,7
63             DO 350 J=1,10
64                 LI(TRI,J,I)=ILDF(I,J) + NLI(TRI,I,J)*B
65 350         CONTINUE
66 400         CONTINUE
67
68         END
69
OF..
EOT..
UP

```

```

LI,1,50
1 *****
2
3 * INTEGRATE OVER SPACE (X), ACROSS THE LOCAL TRIANGLE
4
5     SUBROUTINE SPING(DX,TRI,TRIP)
6
7     PARAMETER (MNODE=151 , MNTRIA=46)
8     DOUBLE PRECISION NLI(MNTRIA,7,10),AS(MNODE*(MNODE-1)/2)
9     DOUBLE PRECISION LI(MNTRIA,10,7)
10    DOUBLE PRECISION UI1(10,10),UI2(10,10),UI3(10,10)
11    DOUBLE PRECISION UI4(10,10),DX(MNTRIA),NLM(MNTRIA,14,10,10)
12    DOUBLE PRECISION ML(MNTRIA,10,10),MG(MNODE,MNODE)
13    DOUBLE PRECISION UI5(10,10),UI6(10,10),UI7(10,10)
14    INTEGER TRI,TRIP
15    COMMON MG,ML,NLM,LI,NLI,AS
16
17 * TAKE PRODUCT OF LI, AND INLF - RECALL LI IS IN
18 * COLUMNS, AND INLF IN ROWS
19     DO 100 I=1,10
20         DO 50 J=1,10
21             UI1(I,J)=LI(TRI,I,1)*NLI(TRIP,1,J)
22             UI2(I,J)=LI(TRI,I,2)*NLI(TRIP,2,J)
23             UI3(I,J)=LI(TRI,I,3)*NLI(TRIP,3,J)
24             UI4(I,J)=LI(TRI,I,4)*NLI(TRIP,4,J)
25             UI5(I,J)=LI(TRI,I,5)*NLI(TRIP,5,J)
26             UI6(I,J)=LI(TRI,I,6)*NLI(TRIP,6,J)
27             UI7(I,J)=LI(TRI,I,7)*NLI(TRIP,7,J)
28 50         CONTINUE
29 100     CONTINUE
30
31
32 * DO WEDDLES N=6 RULE INTEGRATION
33     DO 200 I=1,10
34         DO 150 J=1,10
35             NLM(TRI,TRIP,I,J)=(DX(TRI)/20.0)*(UI1(I,J)+5.0*UI2(I,
36 C +UI3(I,J)+6.0*UI4(I,J)+UI5(I,J)+5.0*UI6(I,J)+UI7(I,J))
37 150         CONTINUE
38 200     CONTINUE
39
40     END
EOF..
EOT..

```

## Appendix H - Spherical Harmonic Angular Fluxes and Data File

### SDATA

This appendix contains the contents of three data files, PNDATA5, and PNDATA9 called to compare finite element angular fluxes in subroutine OUTPUT, and SDATA, a data file called by subroutine GDATA, which contains submatrices of the cubic three dimensional interpolate, as well as integrals of the 20 polynomials used in the three dimensional cubic fit.

The angular fluxes are those computed with 46 legendre polynomials. They are formatted differently in this appendix than in the manner the code of appendix A reads them.

VE  
Pn BENCHMARK DATA WITH 46 LEGENDRE POLYNOMIALS  
FOR c=.5

X	U=-1.0	-.75	-.50	-.25	0.0
0.00	0.5168E-01	0.7383E-01	0.1009E+00	0.1025E+00	0.1213E+00
0.25	0.4860E-01	0.6105E-01	0.7545E-01	0.8841E-01	0.1028E+00
0.50	0.4154E-01	0.4822E-01	0.5639E-01	0.6856E-01	0.8217E-01
0.75	0.3335E-01	0.3746E-01	0.4289E-01	0.5246E-01	0.6354E-01
1.00	0.2628E-01	0.2905E-01	0.3295E-01	0.4038E-01	0.4931E-01
1.25	0.2050E-01	0.2251E-01	0.2544E-01	0.3115E-01	0.3838E-01
1.50	0.1587E-01	0.1742E-01	0.1972E-01	0.2405E-01	0.2986E-01
1.75	0.1223E-01	0.1347E-01	0.1532E-01	0.1859E-01	0.2320E-01
2.00	0.9401E-02	0.1043E-01	0.1193E-01	0.1439E-01	0.1803E-01
2.25	0.7221E-02	0.8074E-02	0.9299E-02	0.1116E-01	0.1401E-01
2.50	0.5548E-02	0.6259E-02	0.7256E-02	0.8665E-02	0.1089E-01
2.75	0.4267E-02	0.4857E-02	0.5666E-02	0.6737E-02	0.8471E-02
3.00	0.3286E-02	0.3773E-02	0.4427E-02	0.5244E-02	0.6592E-02
3.25	0.2536E-02	0.2934E-02	0.3460E-02	0.4086E-02	0.5132E-02
3.50	0.1960E-02	0.2284E-02	0.2705E-02	0.3187E-02	0.3998E-02
3.75	0.1519E-02	0.1779E-02	0.2114E-02	0.2488E-02	0.3117E-02
4.00	0.1179E-02	0.1388E-02	0.1653E-02	0.1943E-02	0.2431E-02
4.25	0.9172E-03	0.1084E-02	0.1293E-02	0.1519E-02	0.1897E-02
4.50	0.7150E-03	0.8466E-03	0.1011E-02	0.1188E-02	0.1481E-02
4.75	0.5585E-03	0.6620E-03	0.7910E-03	0.9292E-03	0.1157E-02
5.00	0.4370E-03	0.5181E-03	0.6188E-03	0.7274E-03	0.9044E-03

X	U=.25	.50	.75	1.0
0.00	0.2755E+00	0.5263E+00	0.7671E+00	0.1014E+01
0.25	0.1821E+00	0.3626E+00	0.5886E+00	0.8265E+00
0.50	0.1300E+00	0.2580E+00	0.4498E+00	0.6647E+00
0.75	0.9471E-01	0.1863E+00	0.3433E+00	0.5328E+00
1.00	0.7029E-01	0.1359E+00	0.2619E+00	0.4266E+00
1.25	0.5301E-01	0.1001E+00	0.2000E+00	0.3413E+00
1.50	0.4042E-01	0.7435E-01	0.1528E+00	0.2730E+00
1.75	0.3104E-01	0.5561E-01	0.1169E+00	0.2182E+00
2.00	0.2396E-01	0.4185E-01	0.8950E-01	0.1744E+00
2.25	0.1856E-01	0.3166E-01	0.6861E-01	0.1393E+00
2.50	0.1441E-01	0.2406E-01	0.5265E-01	0.1112E+00
2.75	0.1122E-01	0.1835E-01	0.4045E-01	0.8878E-01
3.00	0.8743E-02	0.1405E-01	0.3111E-01	0.7084E-01
3.25	0.6821E-02	0.1079E-01	0.2395E-01	0.5649E-01
3.50	0.5326E-02	0.8310E-02	0.1845E-01	0.4503E-01
3.75	0.4160E-02	0.6415E-02	0.1423E-01	0.3588E-01
4.00	0.3252E-02	0.4962E-02	0.1099E-01	0.2857E-01
4.25	0.2542E-02	0.3846E-02	0.8489E-02	0.2275E-01
4.50	0.1988E-02	0.2985E-02	0.6564E-02	0.1810E-01
4.75	0.1555E-02	0.2321E-02	0.5080E-02	0.1440E-01
5.00	0.1217E-02	0.1806E-02	0.3934E-02	0.1144E-01

AD-A159 245

A FINITE ELEMENT SOLUTION OF THE TRANSPORT EQUATION(U)  
AIR FORCE INST OF TECH WRIGHT-PATTERSON AFB OH SCHOOL  
OF ENGINEERING F A TARANTINO MAR 85 AFIT/GNE/PH/85M-19

3/3

UNCLASSIFIED

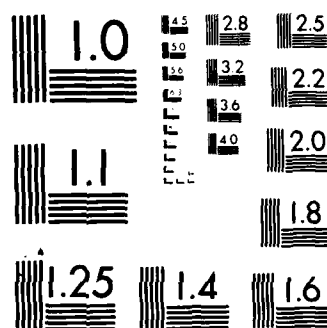
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ONE



MICROCOPY RESOLUTION TEST CHART  
NATIONAL BUREAU OF STANDARDS 1963-A

XE  
Pn BENCHMARK DATA WITH 46 LEGENDRE POLYNOMIALS  
FOR c=.9

X	U=-1.0	-.75	-.50	-.25	0.0
0.00	0.1465E+00	0.1566E+00	0.1708E+00	0.1956E+00	0.2500E+00
0.25	0.1192E+00	0.1322E+00	0.1484E+00	0.1636E+00	0.1915E+00
0.50	0.1039E+00	0.1153E+00	0.1289E+00	0.1433E+00	0.1634E+00
0.75	0.9149E-01	0.1009E+00	0.1121E+00	0.1252E+00	0.1421E+00
1.00	0.8035E-01	0.8826E-01	0.9774E-01	0.1093E+00	0.1238E+00
1.25	0.7049E-01	0.7725E-01	0.8538E-01	0.9549E-01	0.1081E+00
1.50	0.6181E-01	0.6763E-01	0.7467E-01	0.8352E-01	0.9453E-01
1.75	0.5417E-01	0.5923E-01	0.6535E-01	0.7309E-01	0.8273E-01
2.00	0.4746E-01	0.5188E-01	0.5723E-01	0.6399E-01	0.7243E-01
2.25	0.4158E-01	0.4544E-01	0.5013E-01	0.5603E-01	0.6343E-01
2.50	0.3642E-01	0.3981E-01	0.4393E-01	0.4908E-01	0.5557E-01
2.75	0.3191E-01	0.3489E-01	0.3850E-01	0.4301E-01	0.4868E-01
3.00	0.2796E-01	0.3058E-01	0.3374E-01	0.3768E-01	0.4266E-01
3.25	0.2450E-01	0.2680E-01	0.2958E-01	0.3303E-01	0.3738E-01
3.50	0.2147E-01	0.2349E-01	0.2593E-01	0.2895E-01	0.3277E-01
3.75	0.1882E-01	0.2059E-01	0.2273E-01	0.2538E-01	0.2872E-01
4.00	0.1650E-01	0.1805E-01	0.1993E-01	0.2225E-01	0.2518E-01
4.25	0.1446E-01	0.1582E-01	0.1747E-01	0.1950E-01	0.2207E-01
4.50	0.1268E-01	0.1387E-01	0.1532E-01	0.1710E-01	0.1935E-01
4.75	0.1111E-01	0.1216E-01	0.1343E-01	0.1499E-01	0.1696E-01
5.00	0.9745E-02	0.1066E-01	0.1178E-01	0.1314E-01	0.1487E-01

X	U=.25	.50	.75	1.0
0.00	0.3044E+00	0.3292E+00	0.3434E+00	0.3534E+00
0.25	0.2396E+00	0.2817E+00	0.3049E+00	0.3228E+00
0.50	0.1983E+00	0.2387E+00	0.2690E+00	0.2926E+00
0.75	0.1690E+00	0.2041E+00	0.2362E+00	0.2623E+00
1.00	0.1455E+00	0.1757E+00	0.2068E+00	0.2336E+00
1.25	0.1261E+00	0.1519E+00	0.1809E+00	0.2074E+00
1.50	0.1098E+00	0.1318E+00	0.1582E+00	0.1838E+00
1.75	0.9575E-01	0.1146E+00	0.1384E+00	0.1626E+00
2.00	0.8366E-01	0.9986E-01	0.1210E+00	0.1437E+00
2.25	0.7318E-01	0.8713E-01	0.1059E+00	0.1268E+00
2.50	0.6405E-01	0.7611E-01	0.9261E-01	0.1118E+00
2.75	0.5609E-01	0.6654E-01	0.8105E-01	0.9856E-01
3.00	0.4914E-01	0.5821E-01	0.7095E-01	0.8681E-01
3.25	0.4305E-01	0.5094E-01	0.6212E-01	0.7642E-01
3.50	0.3773E-01	0.4460E-01	0.5440E-01	0.6723E-01
3.75	0.3307E-01	0.3907E-01	0.4765E-01	0.5913E-01
4.00	0.2899E-01	0.3422E-01	0.4174E-01	0.5199E-01
4.25	0.2541E-01	0.2999E-01	0.3657E-01	0.4569E-01
4.50	0.2228E-01	0.2628E-01	0.3204E-01	0.4015E-01
4.75	0.1953E-01	0.2303E-01	0.2808E-01	0.3527E-01
5.00	0.1712E-01	0.2019E-01	0.2461E-01	0.3097E-01

ED SDATA

LI,1,35

1 LINES 2-11 U(5,20)

2	6.0	2.0	2.0	2.0	6.0	2.0	2.0	2.0	6.0	2.0
3	2.0	2.0	6.0	2.0	2.0	2.0	1.0	1.0	1.0	1.0
4	24.0	6.0	6.0	6.0	6.0	4.0	2.0	2.0	6.0	4.0
5	2.0	2.0	6.0	4.0	2.0	2.0	1.0	2.0	2.0	2.0
6	6.0	4.0	2.0	2.0	24.0	6.0	6.0	6.0	6.0	2.0
7	4.0	2.0	6.0	2.0	4.0	2.0	2.0	1.0	2.0	2.0
8	6.0	2.0	4.0	2.0	6.0	2.0	4.0	2.0	24.0	6.0
9	6.0	6.0	6.0	2.0	2.0	4.0	2.0	2.0	1.0	2.0
10	6.0	2.0	2.0	4.0	6.0	2.0	2.0	4.0	6.0	2.0
11	2.0	4.0	24.0	6.0	6.0	6.0	2.0	2.0	2.0	1.0

12 SUB MATRICES M5 THROUGH M8 AND M18 OF TETRAHEDRAL CUBIC

13 INTERPOLANT COEFFICIENT MATRIX

14	0.0	0.0	0.0	0.0
15	1.0	0.0	1.0	1.0
16	1.0	1.0	0.0	1.0
17	1.0	1.0	1.0	0.0
18	1.0	0.0	1.0	1.0
19	0.0	0.0	0.0	0.0
20	1.0	1.0	0.0	1.0
21	1.0	1.0	1.0	0.0
22	1.0	0.0	1.0	1.0
23	1.0	1.0	0.0	1.0
24	0.0	0.0	0.0	0.0
25	1.0	1.0	1.0	0.0
26	1.0	0.0	1.0	1.0
27	1.0	1.0	0.0	1.0
28	1.0	1.0	1.0	0.0
29	0.0	0.0	0.0	0.0
30	27.0	0.0	0.0	0.0
31	0.0	27.0	0.0	0.0
32	0.0	0.0	27.0	0.0
33	0.0	0.0	0.0	27.0

EDT..

## VITA

Captain Frederick Angelo Tarantino was born on 25 August 1955 in Hudson Falls New York. He graduated from St. Marys Academy of Glens Falls New York in June of 1973, and continued his studies at Rensselaer Polytechnic Institute, where he earned his B.S. in physics. A Distinguished Military Graduate of that institution's Army ROTC program, Tarantino received a RA commission in the U.S. Army Infantry. Military duties have included mechanized infantry assignments both overseas and CONUS, where he commanded Attack Company of the 2<sup>nd</sup> Bn(M) 34<sup>th</sup> Infantry, Fort Stewart Ga. While assigned to the Air Force Institute of Technology he pursued a Master of Science degree in Nuclear Science. Upon graduation, Tarantino will be assigned as a Military Research Associate at Lawrence Livermore Laboratories, Livermore California. He is a member of Tau Beta Pi. Married to the former Jazmine T. Herrera of Panama, Rep. of Pma., they have two children, Michael John and Monica Maria.

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